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(Broker Inn, Boulder, Colorado, 15-16 February 1995)

Robert M. Banta, Editor

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ABSTRACT. The stockpile of outdated military explosives, ordnance, and propellants is large, dangerous, and growing rapidly. The preferred, most efficient, and most cost-effective method of destruction is the open burning (OB) or open detonation (OD) of the material, but because these methods release contaminants to the atmosphere, a permit from the Environmental Protection Agency (EPA) is required. No routine procedures or guidelines currently apply to OB/OD activities. Therefore, a Workshop sponsored by the Strategic Environmental Research and Development Program (SERDP) and EPA was convened in Boulder, Colorado to discuss regulations and procedures that *do* apply to OB/OD and to discuss potential problems and solutions regarding these methods of destruction. Workshop participants endorsed an enhanced Gaussian puff model using local, recent meteorological input data from a mobile atmospheric observing platform (MAOP), and the characteristics of the model and the observing system comprised the major recommendations of the Workshop. The Workshop emphasized the urgent need for a more accurate characterization of the source, including the amount and nature of materials released, the spatial distribution of the material, the heat released, the noise created, and other relevant quantities. Participants also discussed emerging technologies and capabilities that may be available during the next 3 to 5 years, that could facilitate greatly the ability to address the OB/OD problem.

1. INTRODUCTION

Since the end of the cold war and the scaling back of military operations, unused ordnance and propellants have been accumulating at an alarming rate. Because many of these materials can spontaneously transform into unstable compounds, or become unstable themselves in time, an increasingly urgent need exists to dispose of these stockpiles. An efficient technique is the open burning (OB) or open detonation (OD) of munitions in large quantities (~1-50 tons), and studies indicate that the larger the quantities involved in a single burning or detonation, the more efficient the conversion of the material to stable, nontoxic, end-product compounds. Unfortunately, large-scale OD's produce more noise, lift greater quantities of dust, and release larger quantities of contaminants into the atmosphere and soil. In order to assure that OB/OD operations do not produce human-health or other environmental hazards, organizations wishing to destroy materials in this manner must obtain permits from the Environmental Protection Agency (EPA) before conducting the operations. However, few procedures or guidelines currently exist for the issuing of permits.

The problem of destroying large quantities of ordnance by OB/OD without significant adverse environmental effects is multifaceted, involving operational, regulatory, and combustion chemistry considerations in addition to requiring expert knowledge of the state of the art in specifying and predicting the atmosphere and its role in transporting contaminants. To address these issues a panel of 26 experts in these areas convened at the Broker Inn in Boulder, Colorado

on 15-16 February 1995. The main purpose of the Workshop was to discuss and provide recommendations on a dispersion modeling program and a meteorological platform design that would be used in assessing the environmental effects of OB/OD and in obtaining EPA permits for conducting OB/OD.

The munitions-stockpile problem had been previously addressed by a committee of National Oceanic and Atmospheric Administration (NOAA), Department of Defense (DOD), and EPA personnel under the Strategic Environmental Research and Development Program (SERDP). This group prepared preliminary plans for development of an atmospheric dispersion model using recent findings in boundary-layer meteorology. Recognizing that advances in model physics would produce little improvement without better observational input than is routinely used at present, they also recommended construction of a mobile atmospheric observing platform capable of providing current profiles or soundings of important meteorological variables close to the source. One of the purposes of the Workshop was to assess these prior recommendations. To this end a "straw-man" version of a dispersion model and a design for a mobile meteorological platform (MAOP) was compiled by Dr. Jeffrey Weil and distributed to participants before the Workshop. This straw man has evolved into the paper reprinted in Appendix B.

The goals and objectives of this Workshop were to:

1. Review and discuss the state of meteorological turbulence and diffusion modeling as it might apply to OB/OD permitting.
2. Examine the current capabilities of instrumentation and remote sensing as it relates to the accurate modeling of atmospheric dispersion as applied to OB/OD permitting problems.
3. Consider what new capabilities in modeling and instrumentation may be available in the next 3 to 5 years.
4. Review and assess the straw man dispersion model and proposed meteorological-support instrumentation.
5. Recommend laboratory and field experiments to aid in model development and evaluation.

The Workshop consisted of a mixture of short presentations and open discussions. Following is a summary of issues discussed and brief summaries of the presentations given. Presentation summaries are identified by titles and presenters, followed by indented paragraphs. Questions/answers and other comments as recorded by the rapporteur appear in small type.

2. BACKGROUND

2.1 The OB/OD Problem

2.1.1 OB/OD emissions and the need for modeling (adapted from Appendix B)

The disposal of the demilitarization stockpile---unwanted munitions, rocket propellants, and manufacturing wastes---is necessary at DOD and Department of Energy (DOE) facilities. Disposal methodologies include: 1) recovery and reclamation technology, 2) thermal destruction methods such as incineration and popping furnaces, 3) research stage technology such as electrochemical reduction and biodegradation, and 4) open burning (OB) or open detonation (OD). OB/OD takes place in an earthen pit, trench, or bermed area and is the most common disposal method in use today; this stems from its effectiveness, low cost, and the capacity to treat a wide range of munitions.

The existing demilitarization stockpile is estimated to be about 440,000 tons and is increasing at the rate of about 40,000 tons per year. However, the material destroyed in a single detonation typically ranges only from 100 to 5,000 lb, while the quantity destroyed in a burn ranges from 10 to 10,000 lb. Thus, a large number of detonations or burns will be required to significantly reduce the existing stockpile.

Consideration is being given to increasing the size of individual detonations subject to approval by appropriate regulatory agencies. OB/OD operations generate air pollutants and require predictions of pollutant concentrations to assess air quality impacts and health risks. The pollutants include SO_2 , NO_x , CO, particulates, volatile organic compounds and hazardous or toxic materials such as metals, cyanides, and semivolatile organics. Soil entrained by a detonation is an additional contaminant to consider. Emissions from OB/OD sources have the following special features: 1) "instantaneous" or short-duration releases of buoyant material, 2) considerable variability in the initial cloud size, shape, and height, and 3) ambient exposure times for individual clouds that are significantly less than usual averaging times (typically ≥ 1 hr) of air quality standards.

Predictions of air quality impact require the use of atmospheric dispersion models together with model inputs on source and meteorological conditions. Currently, there is no recommended EPA model to handle the special features of OB/OD sources. The most commonly used approach is INPUFF, a Gaussian puff model. The basic puff framework is suitable for OB/OD releases although the existing INPUFF has several limitations as discussed in Appendix B. As a result, a model development program was initiated under the sponsorship of SERDP. A related program has been acquiring information on OB/OD emission factors from experimental test chambers ("bang boxes") and field studies.

For air quality predictions and assessments, the current focus by EPA and state regulatory

agencies is on the near-source, ground-level concentration (GLC) impact (i.e., exposure to workers and residents at downwind distances within a few kilometers).

2.1.2 "Overview of SERDP and OB/OD operations," Dr. William Mitchell, EPA / AREAL

2.1.2.1. Overview of SERDP. The Strategic Environmental Research and Development Program (SERDP) was established by the U.S. Congress in 1991 as a Department of Defense (DOD) program planned and executed in partnership with the Department of Energy (DOE) and the Environmental Protection Agency (EPA). The goals of SERDP are to:

- address environmental matters of concern to enhance military operations, improve effectiveness of military systems, and help ensure the safety of personnel;
- address defense concerns for reducing operational and life-cycle costs, including those associated with environmental cleanup and costs of full compliance with environmental regulations.

These goals are to be achieved through:

- identifying and supporting programs of basic and applied research and development;
- facilitating environmental compliance, remediation, and restoration activities;
- minimizing waste generation, including reduction at the source;
- substituting use of nonhazardous, nontoxic, nonpolluting, and other environmentally sound materials and substances;
- promoting the maximum exchange of information and minimizing duplication regarding environmentally related research and development activities;
- providing for appropriate access to data under the control of, or otherwise available to, the DOD and DOE that is relevant to environmental matters;
- providing for the identification and support of research and development, and application of technologies developed for national defense purposes that may address DOD matters of environmental concern.

2.1.2.2 Disposal of munitions and propellants. A major concern of the DOD and DOE is the efficient disposal of unneeded or unserviceable munitions and propellants in an environmentally sound but also cost-effective manner. The U.S. Army has 3.8 million tons of conventional weapons in its inventory. Approximately 400,000 tons of this inventory are excess, unserviceable, and/or obsolete munitions and propellants including waste from the manufacture of munitions and

propellants. The amount of excess munitions and propellants is also increasing by 40,000 tons annually. DOE also has 400,000 tons of propellants needing to be destroyed.

Attempts to sell the excess inventory overseas have been unsuccessful. Many items in the inventory cannot be transported to facilities for destruction, and the facilities at which they are stored are facing closure. The traditional and currently predominant method for destroying munitions and propellants is by OB/OD.

To perform open-air burns or detonations at a U.S. facility, requires a permit from EPA. These permits can be very restrictive. For example in 1992, only 4 of 17 U.S. Army facilities could detonate more than 500 lb, and only one facility could detonate more than 3,000 lb. at one time.

In several situations, populated areas have grown closer to the facilities so that toxic emissions, generation of shrapnel, and blast wave effects (i.e., noise and destructive effects) are of critical concern. Methods for reducing OB/OD emissions and shrapnel and mitigating the explosive blast must be developed to dispose of munitions at their storage site and for large-scale OB/OD (25-50 tons at a time).

EPA regulators currently have almost no means of assessing the effects of OB/OD on the environment. The issuing of EPA permits is largely based on extrapolation from small-scale detonations conducted in bang-box facilities or a few larger-scale, open-air detonations. While these demonstrations largely validate certain aspects of the OB/OD technique, many questions regarding large-scale OB/OD cannot be answered in this way.

Specific unanswered questions about large-scale OB/OD activities include the efficiency with which various munitions and propellants--some of which involve casings or packing materials--can be consumed by OB/OD operations. Other questions include the heat generated, radiative loss, and the remaining energy available for plume rise. The entrainment of dust, and the noise and destruction levels of a blast wave for varying amounts or types of munitions are also of concern.

2.1.2.3 SERDP programs on OB/OD. The SERDP program is funding two complementary research and development projects relating to the disposal of munitions and propellants through OB/OD operations. One of these projects, entitled "Characterization of OB/OD Emissions (SERDP Project 94-247)," is being conducted at Dugway Proving Ground, Utah. The goals of this project are: 1) to develop emission factors for the pollutants released when conventional munitions and energetics are destroyed through OB/OD, 2) to obtain information on the physical characteristics of the plumes released from OB/OD activities (e.g., plume shape, plume-size, plume rise-rate, latent heat in plume, etc.), and 3) to find a means to control the pollutant emissions, blast waves, and sound waves generated from OB/OD operations.

Before they had received SERDP funding, researchers at Dugway demonstrated through a series of field and chamber studies that small-scale detonations (220 g) and burns (2,200 grams) in

a 1,000-m³ building (bang box) would yield pollutant emission factors (EF) that simulated quite well the EF which were generated from large-scale OB (3,200 kg) and OD (900 kg) operations. Dugway researchers conducted these tests from 1988 to 1991. These tests showed that when properly conducted, OB/OD activities released relatively low levels of toxic materials that did not appear in dangerous concentrations even close to the site of the OB or OD. They served as the basis for Dugway's and our proposals to SERDP to more fully characterize the environmental soundness of OB/OD activities, and to assess DOD and DOE's capability to accurately predict the quantities and dispersion of pollutants from OB/OD activities.

The other SERDP project, which is the subject of this Workshop, is entitled "Obtaining OB/OD Permits" (SERDP-94-251). EPA has the lead in this project which is being carried out in partnership with the National Oceanic and Atmospheric Administration (NOAA). The goals of this project are to develop a mobile, ground-based profiler that will provide on a continuous basis an accurate profile of the meteorological conditions (e.g., wind speed, wind direction, humidity, atmospheric stability, height of the conventional boundary level, etc.) to 3 km at OB/OD sites; and to develop and field-validate air-pollutant dispersion models that accurately predict how the pollutants released by OB/OD activities will disperse in the environment.

Taken together, these two SERDP projects will provide DOD, DOE, and EPA the tools they need to ensure that OB/OD activities can be permitted and conducted in an environmentally sound manner.

2.1.2.4 Purpose of this Workshop. The purpose of this Workshop is to help us identify the kind of air-pollutant dispersion modelling activity we should pursue, and what kind of observational capabilities will be needed to support the dispersion model or models so that OB/OD permits can be issued with assurance that the health and welfare of human beings and ecosystems is protected.

Q: If there is incomplete detonation, would emissions be higher?

A: Yes, if the detonation is not properly done the emissions would be higher. It is important to arrange the materials to be detonated correctly. Large-scale detonations can be more efficiently carried out, but they can certainly cause large quantities of pollutants to be emitted if they are done in a sloppy or careless manner.

Q: Was (soil) deposition measured at ground level (in the Dugway field tests of 1989-1990)?

A: Yes, the soil that deposited on the ground was collected in 1-m² pans located at 30° intervals on circumferences located at 50, 100, 150, and 200 m from the detonation site. This material was placed in clean jars, extracted, and analyzed for semivolatile organic compounds and for metals. Only very small quantities of these compounds and metals were found.

2.2 Current Regulatory Applications: Approval of Permits for OB/OD

"Current Permitting Procedures," Elizabeth Bartlett, EPA Region IV, Atlanta

Regulations under the Resource Conservation and Recovery Act (RCRA) were promulgated by EPA to address the treatment, storage, and disposal of hazardous waste. These regulations are administered either by EPA or by states authorized to implement RCRA in lieu of EPA. Explosive wastes are considered to be hazardous because they exhibit the characteristic of reactivity under RCRA. Therefore, OB/OD of waste explosives is considered hazardous waste treatment, which requires a permit under Code of Federal Regulations (CFR) 40, Part 264, Subpart X - Miscellaneous Units. Note that Air Permits may also be required but are not included in this discussion.

Unlike other subparts, which contain specific technological standards for units such as tanks and landfills, Subpart X outlines more general environmental performance standards. In order to receive a permit under Subpart X, applicants must demonstrate that miscellaneous units will be "located, designed, constructed, operated, maintained, and closed in a manner that will ensure protection of human health and the environment." Protection includes "prevention of any releases that may have adverse effects on human health or the environment due to [direct and/or indirect] migration of waste constituents" in the groundwater, subsurface environment, surface water, wetlands, soil surface, or air. With regard to OB/OD, evaluation of the air pathway has been the biggest challenge for both applicants and regulators and is the focus of the remainder of this discussion.

Under procedures that have been used thus far in an application for an OB/OD RCRA permit, the applicant prepares and submits a Part B Permit Application for review by EPA and/or the state. The applicant must specify what material is to be destroyed and propose operating conditions or "controls" to be used. The Operating Controls--the conditions and procedures under which the OB or OD would be conducted--include: the amount of the material that will be destroyed at one time, the maximum frequency of such operations through the year, environmental (especially meteorological) conditions under which burns or detonations would be performed, and procedures followed before, during, and after the burn to assure minimal adverse environmental effects. These can include specific climatological or meteorological conditions when OB/OD is allowed, procedures for decision-making that will ensure minimal environmental impacts, and other such considerations. The applicant must then show that when specified quantities of the material are destroyed under the specified Operating Controls, human health and environment (HHE) are protected.

One procedure that has been used for obtaining permits consists of the following steps:

- characterize the emissions
- calculate the dispersion of the emissions to receptor sites under the specified environmental (meteorological, etc.) conditions using an approved atmospheric dispersion model
- demonstrate that risk/exposure assessment is acceptable

Thus, atmospheric dispersion modeling is used in support of the permitting process. In this

role, two considerations are important: the quantity per detonation or burn and the number and frequency of detonations or burns throughout the year. The quantity per detonation/burn is used to show that acute exposures are acceptable for the worst-case meteorological conditions possible under the defined Operating Controls. The number and frequency are required to show that chronic exposures of carcinogens or other toxics are at or below acceptable levels. Acute values are based on short-term exposure, and chronic values are based on the annual average exposure over the lifetime of the OB/OD facility. In the future it is expected that indirect risk by dry or moist deposition processes will also come under scrutiny. Part of the overall assessment may include an analysis of exposures to toxics by groundwater, surface water, wetlands, soil, air, and through other indirect paths.

Typical permit requirements include design, operation, detection, and monitoring of hazardous wastes. A sample of such a permit was developed in Mississippi for a manufacturing-waste OB/OD facility (note: that facility never came into operation).

The most useful output from the models would be isopleths over the local geographical region of concentrations or deposition of pollutant species. These are most readily used in the risk assessment process.

When the modeling shows that the proposed OB/OD operations, conducted under the Operating Controls proposed in the permit application, will be protective of HHE, a final determination is made by EPA. If the permit is issued, the specified Operating Controls become the permit limits, i.e., the conditions and procedures under which the OB or OD is permitted to be conducted.

Q: Why is EPA seemingly biased against OB/OD with preference to incineration?

A: EPA is not convinced that OB/OD can be properly and rigorously characterized and explained, especially as it regards air, but must also address groundwater, soils, etc.

Workshop participants noted that two direct roles for atmospheric dispersion modeling were suggested by this process: as support for the application itself, and as an integral part of the procedure specified under Operating Controls. As an example of the latter, the permit might specify that when a given set of meteorological conditions was met, a model would be run 2 hr before the scheduled OB or OD using current, local surface conditions and profiles of wind, atmospheric stability, and other needed atmospheric variables. If the model predicts that concentrations will not exceed certain limits, then the OB/OD would proceed. In this way, not only would execution depend on general criteria--such as weather dominated by a surface high-pressure system and winds from a certain direction--but also the specific conditions of the day in question would be factored into the decision. A third, more indirect role, primarily for prognostic models, was discussed later in the Workshop, namely, using model output to help in the judicious siting of instrumentation.

"OB/OD Dispersion Models in Regulatory Applications," Terry Brown, EPA Region VIII, Denver

Two large sites in Region VIII, Tooele Army Depot and Hill Air Force Base (both in Utah) perform OB/OD. Hill AFB has done some large-scale explosions, but they were not regulated by

EPA, because the distinction is unclear between what is regarded as OB/OD and what is research and development, part of training, and/or general use of the material.

Q: How hazardous is it to transport the materials? Can we consolidate the accumulation areas?

A: Probably not...there are different organizations; lots of unknown information regarding the wastes; questions of instability; plus issues on interstate transportation, state politics, etc.

2.3 Overview of Proposed Approaches

Atmospheric transport and diffusion models are needed "to support proposed Operating Controls." The role of such models includes: 1) evaluation of conditions under which OB/OD operations could be done (climatologically, statistically, or using hypothetical meteorological conditions), and 2) real-time or individual case-study evaluations of wind-borne pollutant problems, including nowcasts or predictions of atmospheric transport of OB/OD products.

An atmospheric transport and diffusion model requires data input from measurements, including source characteristics and atmospheric conditions such as winds and stability. An important question addressed in the Workshop is, how sophisticated do these measurements need to be? Levels of sophistication are summarized below:

1. Currently, model input may include a wind, temperature, and humidity profile and a surface meteorological observation. The profiles are sometimes from a rawinsonde sounding at the nearest airport, which could be 150 km away and 10 or more hours old, because soundings are taken only twice a day.
2. Hourly (perhaps subhourly) wind and temperature profiles taken on site, using (for example) a radar wind profiler equipped with RASS or balloon ascents. This should be regarded as the minimum acceptable level for reasonable modeling of atmospheric transport, especially if the terrain is complex.
3. Networks of surface stations or profilers, to address spatial variability of the flows.
4. Other state-of-the-art possibilities, some to be explored later in this Workshop, might include scanning or airborne remote-sensing systems. Many of these systems would be used in model validation or optimal siting of instruments to be used in routine operations.

Because the quality of model predictions depends critically on the quality of the input measurements, we need to develop a coordinated modeling-observational system to optimize the ability to determine accurate downwind concentrations of potentially harmful emissions.

Atmospheric transport and diffusion models contain three major components:

1. *Source*: That which is passed off to the dispersion (wind field plus diffusion) model,

including the composition, spatial dimensions (vertical and horizontal) of the pollutant cloud at the beginning of the model run.

2. *Wind field*: Atmospheric winds that carry, or advect, the pollutant cloud. May be simple, such as an assumed horizontally homogeneous wind derived from a single measured wind or profile, or complex, such as a two- or three-dimensional interpolation scheme or dynamic model.

3. *Diffusion*: Effects of turbulent processes that spread the puff and dilute the concentrations of the contaminants/emissions.

These three components will be used to organize the summary of the Workshop discussion, so the presentations in some cases will be presented out of the order in which they were given.

Section 3 addresses near-term approaches using modeling and technology now available, with emphasis on simpler modeling that would be more useful in assembling a system today. Section 4 describes modeling and technologies currently under development or being used in research projects; in some cases they are being tested in operational settings. These new capabilities, which include multidimensional atmospheric models and new remote sensors, should be considered for future systems.

3. ATMOSPHERIC TRANSPORT AND DIFFUSION MODELING/MEASUREMENT SYSTEMS: NEAR-TERM

Two distinctions were made during the Workshop: near-term vs. far-term technologies and short-range vs. long-range transport. The first category pertains to research and technology development. Near-term technologies and capabilities are those currently available that should be considered for the system being built now. Far-term are those currently under development that may be available for a next-generation system in 3 to 5 yr. Progress of these systems, technologies, and capabilities should be carefully monitored for inclusion in future systems.

Short-range transport of airborne material was arbitrarily defined to be <30 km (see Appendix B), assuming that for many applications this would represent transport to the "fence line," i.e., locations on the installation or site performing the OB/OD. Long-range transport (>30 km) would generally carry material off site.

The support system now in the planning and development stages, based on technologies and capabilities currently available or that could be available with a modest investment of resources, consists of a source model, a local wind field based on a sounding and other meteorological data from a mobile atmospheric observing platform (MAOP), and a Gaussian-puff diffusion model with a number of modifications to account for recent developments in boundary-layer meteorology.

3.1 Source characterization

It was recognized at the Workshop that a major ongoing area of research crucial to the success of concentration estimates is the accurate characterization of the source. Specification of the initial height, size, buoyancy, and emissions of the pollutant cloud or puff for the atmospheric dispersion model is a complex problem consisting of many aspects, including composition, meteorological factors, and physical factors.

The composition includes the chemical makeup of the emissions from the detonation or burn, the heat released, and the quantity and makeup (including, e.g., particle size distributions) of material such as dust that is lofted during the event. Contained experiments such as the bang box tests described by Dr. William Mitchell are an important source of information and have provided much of the current information. Bang box results probably represent an upper bound on emission factors, because the confined space for the blast, the comparatively low temperatures, and the small quantities involved most likely produce incomplete detonation/combustion of the explosives. Participants commented that larger tests in the atmosphere would be required to accurately investigate behavior under realistic conditions. Dr. Christopher Biltoft noted that the Army was performing tests at Dugway aimed at better source-composition characterization, as described in Section 2.1.2. Because of the critical importance of including the best available source-composition data in the model, this aspect is viewed as both a near-term and a far-term effort, with research ongoing. The model will be run with current information, and as new data become available the source model will be continually updated.

Meteorological factors strongly affect the initial location and dimensions of the contaminant cloud, including the important aspect of vertical distribution or "plume rise," which is affected by buoyancy of the plume and vertical momentum provided by the explosion. If the dispersion model is sufficiently sophisticated, such as the model proposed by Dr. Jeffrey Weil (Appendix B), then the model should account for these effects. However, if simpler models are used, these effects may need to be accounted for in the source characterization. Advection and spread of the puff are mainly controlled by the wind and turbulence profiles. The distribution in the vertical is a key unknown factor, because in stable regions the atmosphere wind profile is often layered, with significantly different wind directions in adjacent layers that may be only a few tens of meters apart. Thus the amount of material advected in each direction depends on how much ends up in each vertical layer, as discussed by Dr. Gary Briggs in Section 3.2.2. Noting that this is one of the more poorly understood meteorological aspects of this problem, Dr. Weil strongly recommended that research be pursued immediately in this area, and he further urged that laboratory or tank studies be given a high priority. Dr. William Snyder, who has been performing laboratory studies for many years, agreed and said that he was willing to perform the research.

Physical factors affecting the distribution of materials include results of strategies designed to mitigate blast or burn effects, such as the initial configuration or arrangement of the munitions, trench or pit shape and depth, and use of water or fog curtains over the munitions to reduce the propagation of sound and shock waves. The water would obviously reduce the sensible heat content

of the cloud and could also scavenge some of the cloud constituents (e.g., particles). Because these techniques affect the vertical distribution of the material, it is important to fully characterize the effects.

3.2 Atmospheric Transport Model

3.2.1 Wind field model

Short-term plans call for one 924-MHz, wind-profiling radar, or "profiler," with RASS, along with other instrumentation to measure the flow and meteorological variables near the surface. In its most basic form, with one vertical profile of meteorological data, this tacitly assumes a horizontally homogeneous model for the wind field, i.e., that the wind, temperature, and other fields can each be represented by one profile.

3.2.2 Diffusion algorithm

"Straw Man Plan for Developing an OB/OD Dispersion Model," Dr. Jeffrey Weil, CIRES

Two general dispersion modeling approaches are proposed for OB/OD sources: 1) a Gaussian puff and/or plume model for "routine" applications, and 2) a Lagrangian particle approach for research purposes and nonroutine applications. The Gaussian puff model addresses dispersion of a buoyant detonation cloud with source buoyancy included for determining the height and spread of the cloud and the degree of cloud penetration of elevated inversions. The model allows for nonisotropic dispersion, i.e., different cloud spreading rates in the three coordinate directions. In addition to buoyancy, the modeled dispersion accounts for the ambient or planetary boundary layer (PBL) turbulence either through: 1) direct turbulence measurements from the meteorological platform, or 2) parameterization of PBL turbulence using measured or inferred micrometeorological variables, using, e.g., the friction velocity (u_*), the convective velocity scale (w_*), or the PBL height (z_i). The puff model is used to estimate the peak short-time averaged concentration in the cloud and the average concentration over some specified time interval (e.g., 1 hr). Depending on the terrain, the model should be applicable to dispersion over distances up to ~30 km.

For short-duration burns (OB), a time-integrated puff model is being pursued with simplifications added to permit quasi-analytical results. For sufficiently long-duration burns (of an as-yet-undetermined release time interval), the integrated puff approach must reduce to a plume model. The plume model will be included as the appropriate (long time) limiting case in the general puff formulation. The puff model is the first priority of the proposed dispersion modeling effort because of its simplicity, its ease of implementation, and its projected widespread use by the dispersion modeling community. Further details of the initial modeling plan are given in Appendix B.

An important need in developing the dispersion model is experimental data on cloud penetration of elevated temperature jumps and thick elevated inversions capping the PBL. It is highly recommended that laboratory experiments with buoyant thermals be conducted in a salt-stratified tank using a procedure similar to that of Saunders (1962) and Richards (1961), i.e.,

without ambient turbulence. The recommended experiments should be conducted with a constant density stratification and/or a density jump above a neutrally stratified layer, which simulates the well-mixed layer of the convective PBL. In addition, it is recommended that thermal cloud dispersion due to ambient turbulence be simulated using instantaneous releases in a laboratory convection tank.

Overall, the consensus of Workshop participants was that OB/OD should be conducted to the greatest extent possible under daytime convective conditions with strong vertical mixing, as occurs routinely during the warm season in the arid parts of the Western United States. However, because of the urgent need to safely destroy large quantities of potentially unstable materials, decision-makers may need to consider conducting OB/OD activities in locations or at times of the year that do not enjoy the advantage of deep, unstable boundary layers to provide good atmospheric mixing. If such situations arise, OB/OD will need to be conducted under less than optimum meteorological conditions, so some attention should be given to those conditions. We considered two aspects of this problem: 1) With a low-level inversion (especially a nocturnal radiation inversion), sound propagation near the ground would be enhanced, so that the noise of the blast would be more of a problem than during afternoon convective conditions. This could be more or less of a problem, depending on the effectiveness of noise suppression techniques at the source. 2) Meteorologically, diffusion could actually be enhanced under some conditions, as described in the following presentation:

"Puff Model Needs to be Layered," Dr. Gary Briggs, NOAA/ARL, RTP

Large OD's have a number of advantages. Dispersion is greatly enhanced because:

1) The deeper plume penetrates into many different layers of stable air overlying the CBL, 2) mix-down is increasingly delayed in higher layers, and 3) different wind directions often occur in different layers (e.g., largest wind shear under convective conditions is in the capping stable layer).

Rise occurs in ~5 min, with puff growth in this stage but no significant downward dispersion. If the model predicts rise into stable air, or a stable cap over a CBL, it ought to be capable of predicting the fraction of total mass in sublayers of the final rise layer. In the downward diffusion stage, the model should account for different mix-down times in each distinct layer (as the CBL slowly penetrates upward into each one), because each layer will have a different concentration, wind direction, and transport speed from the other layers prior to mix-down.

A primary research need is physical modeling (laboratory, tank) studies to show how a buoyant puff distributes its material when it rises through a CBL into realistic overlying stratifications (not simply a sharp inversion). Also, when the penetration of the stable cap is marginal, how does the intensity of turbulence in the CBL (characterized by w_*) affect the degree of penetration and rate of mix-down?

3.3 Atmospheric Measurements

The committee that provided the original, preliminary specifications for the

modeling/observational system recognized that 1) the first, lowest level of sophistication as outlined in section 2.3 would be completely inadequate, 2) the *minimum* instrumentation needed for adequate support of the model would be local, recent profiles (<1 hr old) of wind and temperature for at least the depth of the atmospheric boundary layer (ABL), and 3) system designers should strive for this to the greatest extent possible. The system would need to be mobile, because optimum siting of the measurement system in complex terrain is not always obvious and might require trial and error, and because it was seen as desirable to test the system in more than one locale. These constraints seemed to dictate a 900-MHz-series profiler. Although it was evident to the committee that this profiling system would be basic to any measurement system likely to be envisioned, other alternatives were discussed. Participants were also asked to recommend modifications and additional measurements or configurations to this basic system.

3.3.1 Basic profiling system

"Mobile Atmospheric Observing Platform (MAOP) and Instrument Development" -Brian Templeman, ETL

As part of the SERDP project requirement, a meteorological monitoring platform will be developed and built to serve two purposes: to provide data for input into the OB/OD dispersion model, and to monitor meteorological conditions immediately prior to the OB/OD and ensure that they remain within the Operating Control limits. The initial design was developed by Brian Templeman and Dr. John Gaynor to provide a mobile, easily upgradeable platform that would initially provide the dispersion model with a set of meteorological inputs equaling or exceeding the minimum required. The design of this system was then to be reviewed by peers at the first SERDP Workshop.

The original design of the meteorological monitoring platform included measurements needed for diffusion predictions concerning OB/OD releases through heights actually achieved by OB/OD activities. These include: surface wind speed and wind direction, surface air temperature, relative humidity, solar radiation, barometric pressure, near-surface turbulence values, sensible-heat flux, momentum flux, profiles of wind speed, wind direction, temperature, and the mixing height z_i . The mobile monitoring system will provide two modes of operation. The first mode is the acquisition of meteorological variables and the development of a data base that will aid in the refinement of the dispersion model. In the second mode, the platform will provide the dispersion model with a near real-time meteorological data set that will be used to determine go/no-go decisions for OB/OD activities.

The initial design of the system was intended to implement a flexible, upgradeable approach that could expand with the dispersion model's requirements as it becomes more complex. At the time of the original design, it was unclear what modeling approach would be used, and therefore the exact data requirements were not obvious. However, we now have a better understanding of the model's characteristics and can begin to develop a more detailed system design.

The first step of this redevelopment occurred at the present SERDP Workshop, where the initial design of the mobile monitoring platform was provided to the Workshop attendees. The design was reviewed and refined. Because the Workshop provided a valuable peer-review

environment; some initial decisions could be made as to the scope of the monitoring platform.

At a minimum, the platform will consist of an integrated 924-MHz radar/sodar/ RASS profiling system; a laser-based, mixing-height monitor; several portable mesonet stations (PAMS) with sonic anemometers, temperature, humidity, pressure, and solar radiation sensors. A box van and trailer system will transport and house the monitoring system, which will contain two workstation-class computers. The first Unix-based workstation will be used as a data-ingest computer, and the second will run the OB/OD dispersion model.

"Vertical Resolution of the MAOP: Wind Profiler and RASS Characteristics," Dr. James Wilczak, NOAA/ETL

The characteristics of 900-MHz-class UHF wind profilers with radio-acoustic-sounding system (RASS) were discussed. These profilers typically provide data every 60 or 100 m; however, these data are twice oversampled, so the true vertical resolution is 120 or 200 m. The average maximum heights to which useful data are obtained are typically 2 km for wind and 1 km for RASS temperatures. However, there is great variability in these heights, depending on weather conditions. Mean wind and temperature profiles have historically been generated every hour (55 min of averaging time for winds and 5 min for temperatures). Shorter averaging times can be used to generate the mean profiles, although they may have a lower accuracy. Also, the relative averaging time of temperatures and winds can be varied to give greater accuracy for temperature.

Workshop participants were concerned about whether the 900-MHz-series profilers would provide temperature data to sufficient heights to capture the inversion level structure in a daytime convective boundary layer. Although it was recognized that this was a possible shortcoming, the only remote-sensing alternative is to use a lower frequency profiler, such as a 449-MHz system. Drawbacks of these profilers, however, include their lack of portability, lower vertical resolution, and *considerably* greater cost. When these factors are taken into account, the 449-MHz system is not a feasible alternative for the profiling system.

Another alternative discussed for some experiments was supplementing the 924-MHz profiler with radiosonde ascents; this remains a possibility.

"Technical Characteristics of the Profiler System," Dr. Robert Weber, NOAA/ETL

The MAOP being developed at ETL is similar in many respects to a mobile profiling system (MPS) that was developed recently for the Army Research Laboratory (ARL) at White Sands Missile Range. For example, ETL is building the platform with a modular approach, most of which consists of off-the-shelf technology. Diverse instrumentation was assembled for that platform within 6 months.

The 924-MHz wind/RASS profiler being procured for the MAOP is expected to provide temperature measurements up to 1.5 km above ground level (AGL) depending upon meteorological conditions. That height estimate is based upon experience with existing radars. But this radar is

being integrated with a sodar, whose steerable acoustic source is also used as the acoustic source for RASS. Hence, steerable RASS is an option in future operations with this radar. Steering the acoustic beam may compensate for high winds, which limit coverage with existing nonsteerable acoustic sources. In addition, the power can be boosted on the radar to improve sensitivity. Currently, Radian Corporation is developing a higher-power, integrated piezoelectric/rf antenna system for combined wind/RASS operation. Therefore, it should be possible to increase the profiler coverage for both wind and RASS measurements, even operating at 924 MHz. Therefore, to achieve greater height coverage for the RASS temperature profile, it may be unnecessary to consider using a 449-MHz radar, unless the more sensitive 924-MHz radar is incapable of getting temperature measurements high enough for modeling needs. In any case, we should not consider ourselves limited in coverage at this time. If the potential need for greater coverage indicated in the Workshop does indeed materialize in the future, then options exist for increasing that coverage.

3.3.2 Input required for current-generation model

- Meteorological observations
 - ▶ Mixing height
 - ▶ Wind profiles
 - ▶ Temperature profile structure
 - ▶ Surface heat flux
 - ▶ Surface friction velocity
 - ▶ Inversion strength/wind shears
 - ▶ Turbulence
 - ▶ Humidity profile
 - ▶ w'^2 , w'^3
- Source characterization
 - ▶ Blast (burn) amount and chemicals
 - ▶ Heat released
 - ▶ Source temperature
 - ▶ Cloud temperatures
 - ▶ Chemistry of particulates/gas/condensation
 - ▶ Secondary effects of dust amount and size; shock wave (sound); heat (radiative loss)
 - ▶ Cloud size (there can be considerable disagreement on volumes; may need to use a mass balance to get to it)
 - ▶ Source "shaping" due to design of pits
- Vertical and lateral pollutant mass distribution, within and above the mixed layer, at release and downwind as a function of time (for validation)

3.4 Model Evaluation

Once a modeling/measurement system has been developed, it will be necessary to evaluate its performance in determining contaminant concentrations. During this evaluation it is also desirable to assess how the modeling system could be improved (i.e., to determine the major sources for error).

In performing evaluations of the modeling/measurement system, two classes of instrumentation would be used: those available routinely from the MAOP, and those used to supplement MAOP measurements during the evaluation tests. The purpose of the tests is to determine how well the model, combined with the routine measurement system, can determine the transport of atmospheric contaminants. Secondary objectives would include verification of model components such as the plume-rise portion of the model, derived from tank and other laboratory experiments. Field tests should be done using tracer experiments, but runs should also include actual OB/OD's because of the unusual behavior of the source (e.g., explosion plus buoyant rise of the cloud).

Supplementary instrumentation will provide: 1) finer spatial or temporal resolution of quantities already measured by the MAOP, 2) quantities different from those measured by the MAOP to enhance understanding of physical processes, or 3) a broader view of what the model should be simulating. The first kind of enhancement might include a greater number of surface mesonet stations or profilers in the network. The second would most likely require in situ air-chemistry samplers, and might also include turbulence measurements, additional chemistry measurements, or turbulent flux measurements. The third enhancement might include scanning remote sensing instruments such as Doppler lidars, aerosol-backscatter lidars, or chemical species (DIAL) lidars to map out the flow field or the size, shape, and spatial dimensions of the tracer or contaminant plume as a function of time. Instruments of all these types have proven valuable in research experiments.

3.5 Remaining Problems: Flows over Complex Terrain, Other Complications

Low-level flows encountered in the atmosphere are often too complicated to be represented by a single profile, especially in complex terrain. Complex-terrain flows include mountain-valley and slope winds, sea and lake breezes, and circulations arising from horizontal variations in land use and soil moisture. The following section describes flows encountered in hilly or mountainous terrain.

"ASCOT Program and Complex Terrain Flows," Dr. C. David Whiteman, Battelle Pacific Northwest Laboratories

Air pollution dispersion in valleys differs from dispersion over the plains. Vertical and horizontal dispersion in a valley are enhanced by the increased turbulence associated with the rough underlying terrain. The existence of local flows often keeps the air from stagnating, and better plume rise may occur in the light valley winds associated with thermally driven local circulations. These

factors enhance the dispersive characteristics of the valley atmosphere relative to the plains atmosphere. On the other hand, valleys suffer from having narrow wind roses, so that pollutants are often carried up and down the same paths. Repeated fumigations along these paths or repeated plume impactions on surrounding high terrain can produce high ground-level concentrations. Also, because of the inverse dependence of pollutant concentration on wind speed, pollutant concentrations in valley plumes can be quite high when the plume is emitted into weak, thermally driven, along-valley flows. Weak dispersion associated with stable atmospheric conditions can persist longer in valleys because of the nocturnal drainage of cold air into the valley and the late sunrise and early sunset within the valley caused by shading from the surrounding higher terrain. The evolution of the wind and temperature structure in valleys is quite different from the well-known evolution over the plains. In particular, temperature inversion buildup and breakup involve multiple layers of wind structure, and each of these layers is associated with a temperature structure layer. During the inversion breakup period, for example, heating of the sidewalls produces a warm layer over the sidewalls containing upslope flow.

At the same time, the convective boundary layer growing slowly over the valley floor contains up-valley winds blowing up the valley floor. The remnants of the nocturnal inversion, called the stable core, are usually still present at this time in the center of the valley atmosphere and contain down-valley winds that continue long into the inversion breakup period. Observations on the valley floor typically indicate a weak up-valley flow when the flow in the elevated stable core is actually blowing in the opposite direction--often with considerable speed. Furthermore, because of the nocturnal drainage of cold air into the valley from the surrounding high terrain, an unstable boundary layer can grow very quickly above the ridgetops where the atmosphere is much less stable than over the valley floor.

One of the key problems affecting air pollution dispersion in particular valleys is the lack of suitable techniques to predict the strength of the along-valley wind system. Recent research, however, suggests that along-valley wind system strength may be closely related to the shape of the valley cross section and its change with down-valley distance. Moreover, air pollution dispersion in valleys is complicated by cross-valley flows that develop when one sidewall is more strongly heated than the opposite sidewall. A cross-valley circulation blows toward the more strongly heated sidewall, where fumigations of elevated plumes can occur. Other complications include the effects of terrain constrictions along the course of a valley that isolate low-lying segments of the valley into cold air lakes, and the effects of strong ambient winds above a valley on the local thermally driven circulations that form within the valley. Strong synoptic-scale pressure gradients, when superimposed along the longitudinal axis of a valley, can produce along-valley flow components that are stronger than the locally driven circulations, and this effect is especially pronounced in shallow valleys in moist climatic regimes. The wide variety of complex-terrain phenomena affecting air-pollution dispersion is becoming better known through ongoing research, giving us better insight into how to design measurement networks for the characterization of atmospheric dispersion in complex-terrain areas and how to evaluate and improve existing complex-terrain air quality models.

"Some Problems with Modeling over Complex Terrain," Dr. Robert M. Banta, NOAA/ETL

In modeling dispersion over complex terrain, correctly modeling the advecting wind field is of paramount importance. Two ways in which a wind field can be in error are: 1) when significant amounts of atmospheric contaminant material are advected by flow features that are too small to be sensed by the observational network used for a diagnostic (i.e., interpolation) model (or other model that relies on measurements), and 2) when terrain-forced or other mesoscale flow systems are too large to be properly represented by a model of limited domain.

The first kind of error was observed during a field project at the Rocky Flats Plant (RFP) just east of the Front Range of the Colorado Rockies (Banta et al. 1995, 1996). A nocturnal jet of cold air was observed by ETL's Doppler lidar exiting a canyon ~10 km to the northwest of RFP. This outflow or exit jet formed, strengthened turning southeastward over RFP, and dissipated in a 3- to 4-hr period. While the jet was strong it remained narrow (< 3 km wide) between RFP and the canyon and reached speeds of 3 to 4 m s⁻¹ near the surface. However, it was poorly sampled by the mesonet of surface meteorological observing stations, and thus was poorly represented in the diagnostic flow models used to determine the dispersion of SF₆ tracer released at RFP. The measured tracer distribution indicated a primary plume carried to the east-northeast by the basic surface flow, and a secondary plume to the southeast due to the canyon exit jet. The diagnostic models did a reasonable job of representing the primary plume but missed the secondary plume because of the absence of the exit-jet flow in the diagnosed wind field. This study also showed that significant changes in the structure of the flow field occurred over 30- to 45-min intervals, implying that hourly sampling of the winds or contaminant concentrations are often inadequate.

The second kind of error mostly applies to models attempting to predict future wind fields. An example of conditions under which this is apt to occur were also observed during the Rocky Flats project (Banta et al. 1995). In the regions to the north of Denver, including RFP, a topographically forced mesoscale vortex can form under southeasterly large-scale flow. The flow induced by this vortex can control the low-level wind field in the basin north of Denver, which has a north-south dimension of 100 km. If one wished to *predict* at high resolution (as might be required to simulate a small-scale jet as in the previous paragraph) the flow in a 30-km square, for example, around RFP, this square would be embedded in the regions affected by the vortex. A model too simple or with a domain too small to simulate the vortex would be unable to predict the proper wind field, in spite of the fact that on a larger scale this flow is predictable in principle. What is required, therefore, is either nesting within a larger model of a scale capable of simulating the vortex, or time-dependent boundary conditions representing the evolution of the vortex.

Numerical modeling usually represents a tradeoff between resolution and coverage of the domain. The two limitations described above represent important considerations at both ends of the modeling scale.

Effects of sea/lake breezes are discussed by Dr. Roger Pielke in Section 4.1.1.2. We also discussed the importance of considering other complications such as clouds and fronts.

Q: Do we always consider only clear weather conditions? Some areas can be cloudy most of the time, and we need to consider that.

4. ATMOSPHERIC TRANSPORT AND DIFFUSION MODELING/MEASUREMENT SYSTEMS:

FAR-TERM

To address the deficiencies noted in the previous section, it is necessary to improve models and measurements by considering maturing technologies that may be available operationally in the next 3 to 5 yr. As described previously, improvement of source characterization is regarded as an ongoing need, so the following section will focus on meteorological modeling and measurements. A major area where improvements are noted is in computer workstations, which are becoming better, faster, and less expensive, so that it is conceivable that a prognostic, dynamic 3-D model could operate in the field. Currently, NOAA's Forecast Systems Laboratory (FSL) runs a version of one such model, RAMS, daily to predict airflow patterns and precipitation over Colorado in a setting that mimics operational. Other, similar applications exist as described below. Another major area where technology is rapidly developing is in remote-sensing instrumentation, such as lidar, radar, acoustic-based, and radiometer systems. All of these technologies are becoming more efficient, easier to operate, and less expensive, so they should be watched closely.

4.1 Models

4.1.1 Wind-field models: Multidimensional models

4.1.1.1 Diagnostic: Diagnostic models are essentially interpolation schemes that rely on current measurements to determine the wind field. Some diagnostic algorithms have limited flow physics in the flow calculations. These models are fast but have no inherent predictive capability. Although they have been used for many years, the aspect of their development being considered "far-term" is that they require a more complex interaction with the measurement network and/or remote sensing systems than is currently available. Such models are presently being run operationally for a number of applications, but this model-measurement interaction aspect of development is seen as a far-term capability.

"High-Resolution Modeling," Dr. Ronald M. Cionco, U.S. Army Atmospheric Sciences Laboratory, White Sands Missile Range (WSMR)

For many complex-terrain applications of interest to the U.S. Army (including OB/OD activities at WSMR), a high-resolution, gridded wind field is needed that can be displayed quickly using computational resources equivalent to a personal computer. At present these applications require a diagnostic model with an appropriate graphics package. An example of such a diagnostic model is the high-resolution wind (HRW) model run for many years at WSMR (Cionco 1985). The model is run over domain sizes ranging from 2x2 km to 20x20 km, and it is often embedded in a larger-scale wind field or model. With 50 grid points along each side, resolutions range from 40 to 400 m. Minimum input is one surface observation and one profile of winds, temperature and pressure, but obviously results greatly improve when a network of surface and/or upper air measurement systems is used. HRW interpolates the measured winds to the model grid and then adjusts the wind field to the topography, taking into account whether the earth's surface is cold or warm (i.e., whether the atmospheric surface layer is stable or unstable). The model also accounts

for changes in land use and vegetation as they affect the flow.

A 5x5 km version of HRW with 100-m resolution was recently employed during the recent MADONA diffusion measurement program in England. Examples of model output based on this dataset have been presented by Cionco and Byers (1995). They include horizontal x,y plots of u, v, and vector wind fields, streamlines, potential-temperature, friction-velocity, power-law-exponent, and Richardson-number fields.

4.1.1.2 Prognostic: These models can forecast wind/concentrations, but need greater computer resources

"Use of Prognostic Meteorological Models to Assess the Transport and Dispersion of Atmospheric Emissions," Dr. Roger Pielke, Colorado State University (CSU)

CSU's Regional Atmospheric Modeling System (RAMS), linked to a Lagrangian particle diffusion model, has been applied to several dispersion problems on different scales, including complex terrain. In nested mode, the outer domain of RAMS typically covers a large modeling region in order to include synoptic-scale motions. Nesting down to high spatial resolution allows the model to resolve mesoscale and local-scale circulations and other features. Validation of this modeling system was performed using CAPTEX and Great Plains tracer experiments and, more recently, using tracer data from the Lake Michigan Ozone Study (LMOS). This last study demonstrated the importance of the vertical motion field, produced, for example, by a local circulation such as a lake or sea breeze, in properly predicting the transport of pollutants. Lagrangian particles advected only by the low-level wind field at the level of the source (50 m AGL) were advected a short distance, whereas particles that were allowed to be advected by the full 3-D winds traveled upward to heights of 1.6 km AGL in the lake-breeze convergence zone and carried far to the north with the stronger winds at that level, where they could be fumigated downward to the surface (Lyons et al. 1995; see their Fig. 3). The plume carried by the low-level wind field resembles what would be predicted by many current EPA-approved regulatory models driven by a diagnostic wind-field model. The plume transported by the full 3-D wind field was in good agreement with observations, which showed high concentrations of ozone more than 100 km north of the source.

RAMS is currently being used operationally on a workstation as part of the emergency-response system at Kennedy Space Center to provide 24-h weather forecasts. In the case of a hazardous material release or aborted vehicle launch, this forecast is used to simulate dispersion with the Hybrid Particle and Concentration Transport (HYPACT) model. The scale, resolution, and length of time needed for a forecast are similar to that which would be needed to support OB/OD operations.

These applications, and those described recently by Poulos and Bossert (1995) using data from the Rocky Flats experiment, show that prognostic models can be used effectively over the limited domain sizes required for OB/OD activities. These models have the further advantage that they can be nested within a model of larger scale, enhancing their usefulness as predictive tools. The versatility of RAMS and other predictive models is illustrated by their ability to simulate flow and

dispersion over much larger domains with skill. The following presentation demonstrates this skill in simulations of the effects of regional-scale sources in the southwestern United States on pollution in the Grand Canyon. An interesting and potentially useful modeling tool is the calculation of *influence functions*, which attribute the percentage of pollution at a point in the modeling domain to each of the sources in the domain.

"Project Mohave, Daily Dispersion Simulations," - by Dr. Marek Uliasz, CSU

Another dispersion study with RAMS includes meteorological and dispersion simulations of air pollution in the southwestern United States being performed on workstations for all of 1992. This study focuses on assessment of contributions from local power plants and distant emission sources (e.g., the Los-Angeles-basin area source) to air pollution and visibility in Grand Canyon National Park. The output from RAMS is used to run a simplified version of the Lagrangian particle model in a source-oriented mode to calculate influence functions for a given receptor. A tracer of opportunity (methylchloroform from the Los Angeles area) was used for a preliminary validation and comparison with other simpler modeling approaches. The results from RAMS show higher correlation with observations than the results from the Atmospheric Turbulence and Diffusion (ATAD) model. Dispersion calculated using RAMS also results in greater dispersion from an effluent source than obtained using ATAD. RAMS includes a higher temporal and spatial resolution of the horizontal winds than ATAD, in addition to the effect of vertical motion. On other model runs, dispersion models using wind fields from the Nested Grid Model (NGM) issued by the National Meteorological Center (NMC) provided a negative correlation with observations due to the low resolution of this operational synoptic-scale model.

Relevance to the OB/OD problem:

- Mesoscale meteorological models (such as RAMS) linked to Lagrangian particle models show high skill in simulating dispersion in complex terrain--both in local and in larger than local scale--where simpler models are not applicable. These models are now affordable, because they can be run on dedicated workstations.
- Possible applications for OB/OD operations:
 - Numerical simulations to assess whether the potential impact of OB/OD operations could extend beyond a local scale
 - Numerical simulations to help design the OB/OD operations, including optimization of the siting of the meteorological instrumentation
 - Local weather forecast for specific sites
 - to be used in operational planning for OB/OD
 - to provide meteorological data required by local dispersion modeling not available from local meteorological observations

4.1.1.3 Prognostic with data assimilation: Another application nested down to the OB/OD scale is the use of the RAMS predictive model with 4-D data assimilation (4DDA), in which measured wind (and other meteorological) fields are used to update the model run as observations become available. These models enhance the accuracy of diagnostic models at the "current" time level by ensuring that the modeled fields are consistent with the governing equation set, and then combine this current-level accuracy with the predictive capability of prognostic models. These advantages are gained at the expense of a larger, more complicated (and thus slower) model.

"Multi-scale Data Assimilation in Complex Terrain" - Jerome Fast, Pacific Northwest Laboratories

The RAMS model with a Lagrangian particle dispersion model (LPDM) was used to examine the small-scale circulations influenced by terrain and their effect on dispersion along the Front Range of the Colorado Rocky Mountains in the vicinity of the Rocky Flats Plant (RFP). A nested grid approach was used in RAMS to resolve the topography around RFP. The results of the modeling system were evaluated using meteorological and tracer data collected during four nocturnal periods of the Atmospheric Studies in Complex Terrain (ASCOT) field experiment in January and February 1991. Several other modeling systems made dispersion simulations for these four periods as well, including MATHEW/ADPIC, ATMOS1/ATMOS2, LSDM, TRAC, and RAMS/LPDM (in other configurations); a rigorous intercomparison of the model results has not yet been completed.

The RAMS and LPDM models were able to reproduce some of the unusual dispersion patterns found during the ASCOT field experiment (Fast 1995). For instance, the modeling system and the SF₆ samplers indicated that the tracer plume were probably affected by canyon jets. When a 4DDA technique based on "nudging" was incorporated into RAMS, both meteorological and tracer results were in better agreement with the observations than in runs without 4DDA, as expected. To demonstrate this, predicted wind fields with and without data assimilation were shown for an afternoon and an evening period. While RAMS alone was able to qualitatively capture the flow features, errors still occurred in small-scale features near the foothills of the Front Range. 4DDA reduced errors in the predicted 3-D mesoscale flow fields.

4.1.2 Diffusion scheme

"The Gaussian Puff Model SCIPUFF," Dr. R. Ian Sykes, Titan Research and Technology, Princeton NJ

Gaussian puffs provide an efficient method for tracking the transport and diffusion of a contaminant species. The classical Gaussian puff framework has been extended to describe complex flow effects and nonlinear interactions. The Second-order Closure Integrated Puff (SCIPUFF) model uses turbulence closure theory to represent diffusion, and a generalized moment tensor to describe wind-shear distortion. A splitting/merging scheme provides accurate calculations of complex flows. In addition, the nonlinear calculation of concentration fluctuation variance provides a basis for describing buoyant rise dynamics and nonlinear chemical reaction.

This diffusion algorithm is based on elliptical Gaussian puffs. When the puffs become too

distorted and their eccentricity exceeds a threshold value, the algorithm splits the puffs into two or more puffs, conserving mass of the contaminant (Sykes and Henn 1995). Conversely, a merging scheme combines two puffs when appropriate. The model splits the puff on a grid, and resolves it into the number of puffs needed to describe the concentration field. In one case the model spawned 20,000 puffs. Advantages of the SCIPUFF algorithm are that it is relatively fast, especially when compared with Lagrangian particle type schemes, and highly accurate. As an example, a perspective view of a plume isosurface around a circular hill was shown. The contaminant cloud stretched and went around the hill, and merged back together on the downwind side.

Other sophisticated examples of diffusion schemes are the Markov LPDM algorithms employed in conjunction with RAMS and other predictive models. These schemes were mentioned in Section 4.1.1.2 by Drs. Pielke and Uliasz and Section 4.1.1.3 by Dr. Fast.

4.2 Observational Capabilities

A number of techniques have been developed that could significantly improve the quality of the meteorological data available as input to the model, even in real time. Although these technologies would probably be best suited for focused, larger-scale model verification programs over the next few years (see Section 3.4), commercial, affordable systems are being developed and should be watched for possible inclusion into the modeling/observation system in the future.

- ▶ Networks of profilers and surface stations with 4DDA: Improvements most helpful in this area are the speed of the computers and analysis software, and the development of faster, more efficient algorithms for assimilating real-time data into dynamic, mesoscale model runs. This could make it feasible to deploy accurate models into the field to aid in real-time decision making.
- ▶ Remote sensing instrumentation

Profiler and RASS: New profiling systems with improved acoustic sources are under development, as described by Dr. Weber in Section 3.3.1. These could provide more accurate winds and temperatures, and to greater heights.

Radiometers: FTIR and other radiometer technologies show great promise for detecting and identifying a wide range of airborne pollutant species.

Aerosol backscatter lidars: Scanning lidar systems that detect aerosol clouds are currently in use for research applications. Such systems could directly monitor and map out the location of the contaminant plume for model verification, forecast improvement studies, or be used in case emergency response measures were needed. Development of safer, more stable, and less expensive laser sources optimized for atmospheric work is presently a very active area of research.

Chemical species lidars: Lidars using differential absorption (DIAL systems) and other techniques can currently measure concentrations of gaseous atmospheric pollutants such as ozone in the atmosphere. These instruments are now used in research experiments but will be more user friendly and probably commercialized in the near future. Development of new laser sources and techniques will allow other chemical species to be detected.

Doppler lidar: Scanning Doppler lidars have been used in atmospheric research in complex terrain for several years (see Banta et al. 1995). They are capable of mapping out a wind field in a region of interest, and tracking the aerosol backscatter of the contaminant cloud. More compact, more user-friendly, less expensive systems are under development, and they may be commercially available within the next decade.

5. OTHER ISSUES ADDRESSED

Long-range transport. A potentially significant issue arose in discussing long-range (>30 km or off-site) transport. A perception apparently exists among potential applicants that even *considering* long-range transport may be equivalent in the minds of regulators to admitting that pollutants will be carried off site in potentially dangerous concentrations. Permit applications would thus be automatically rejected.

If true, this situation would be unfortunate, because a consensus of those at the Workshop who deal with transport in complex terrain agreed that conditions will occasionally exist when the contaminant plume spreads little and material can be carried off site in harmful concentrations (e.g., under stable conditions or shallow mixed layers with considerable vertical penetration of the pollutant plume or puff). It is important to be free to consider this possibility and to be sure that it will not happen under Operating Conditions specified in the permit. The objective of this process ought to be to openly consider the effects of long-range transport and to demonstrate that contaminant concentrations will not exceed acceptable levels when OB/OD's are conducted under these Operating Conditions. This would seem to be a case where understanding on the part of both regulator and applicant is necessary to define conditions under which OB/OD's can be carried out with minimal impact, especially considering the hazards of continuing to store large quantities of unstable compounds.

Prognostic models. Roles for 3-D, dynamic mesoscale Numerical Weather Prediction (NWP) models (such as RAMS and MM5) at fine resolution was a topic of controversy. In the past these models ran on big mainframe computers, took many hours to run, and even then produced crude results at relatively coarse spatial resolution. More recently, however, hardware improvements and optimization of model software allow models to run on dedicated workstations, producing fine-resolution wind fields in 1 to 2 hr. Models have been used by NOAA/FSL for forecasting applications and by NASA at Cape Canaveral (as described by Roger Pielke in Section 4.1.1.2). It seemed to some participants that such a tool should be useful in the real-time, decision-making process in determining whether to conduct an OB/OD.

Other Workshop participants did not envision such a role for mesoscale dynamic models. Instead, they felt that such models would be highly useful in defining flow regimes for optimum deployment of instrumentation and in performing sensitivity studies aimed at clarifying what variables need to be measured at what locations and to what accuracy, in order to improve diagnosis or prediction of plume transport. Dr. Dennis Thomson of Pennsylvania State University added that current technology exceeds some needs, but is deficient in others, and that models could be used to help focus on areas of technology development that would produce the greatest improvements in the model/measurement system performance.

Conservatism of estimates. Because of the many uncertainties in representing atmospheric advection and turbulence effects, it is desirable to introduce some conservatism into concentration estimates. Participants discussed how this should be handled in the model--for example, should diffusion be constrained so that calculated concentrations would err on the high side? They felt that conservatism should be represented in the estimates of source strength, and meteorological processes should be represented as accurately as possible. The goal should be for the meteorological models to be unbiased in their characterization of dispersion. Ms. Bartlett pointed out that the more accurately the processes and variables are known and specified, the less is the need for conservatism.

Project responsibility. During the project prior to the Workshop, funding sometimes appeared and needed to be obligated quickly. Decisions, such as whether to procure the profiler/sodar system, were made by a consensus of the committee of ETL, DOD, and EPA personnel, but clear lines of responsibility and management structure had not yet been established. Workshop participants expressed concern for this situation and offered a number of suggestions, including (as summarized by Dr. Thomson):

1. Establish a point of contact for collection and dissemination of OB/OD-related information. (Gennaro (Jerry) Crescenti has since taken on this responsibility.)
2. Appoint a reasonably senior scientist to direct the overall effort and make difficult priority decisions when resources are limited. This person should have a good grasp of the cross-disciplinary issues (theory, modeling, measurements, etc.) and be reasonably independent (i.e., not associated with laboratories or industrial groups that might end up being subcontractors).
3. Consider having a small (perhaps three) interdisciplinary "executive advisory committee" to work with and advise the project director.

Bill Petersen said these suggestions would be taken into consideration after the Workshop in deliberations concerning the most workable management structure for this project.

Differences between OB and OD were not really considered in detail at the Workshop. We generally assumed we were talking about contaminant clouds or puffs from open detonations. At some point, differences for open burning operations should be considered.

5.1 Specific recommendations

Make initial project investments toward better defining the problem. Use and apply existing databases and models to define the experimental needs before constructing and deploying new equipment. People from ETL, EPA, Dugway, White Sands Missile Range, etc., should work together to exploit available resources and to define system and data processing needs and deficiencies.

Provide meteorological and other instrumentation to document OB/OD's currently being carried out. Design a few carefully controlled experiments (e.g., at Dugway) that will help resolve the manifold outstanding questions regarding source characteristics.

Proceed with the development of the MAOP. Include as many additional measurement systems as cost allows. Consider a network of surface stations to document horizontal variability.

Proceed with the development of the diffusion model.

6. SUMMARY: FINAL SESSION

The final session included presentation of a summary outline of the Workshop by NOAA's John Irwin, followed by discussion and recapitulation of issues that participants thought were especially important or had received insufficient attention during the course of the Workshop. The summary outline was presented for participant comment and suggestions, and a final form was adopted.

Particular issues the group thought important were then discussed. These included:

- ▶ Clarification of source characterization, particularly as it relates to the geometry of the detonation. It was commented that "true-scale" experiments need to be conducted; that bang box data cannot be extrapolated to answer all the questions at hand for OB/OD.
- ▶ Immediate design needs of the MAOP, and what will be available in the 3- to 5-year range.
- ▶ Vertical penetration of the puff or plume (raised by Jeff Weil). The key variable is the height of the potential-temperature "jump" with height, because the radius of the thermal grows in proportion to the rise. However, a jump is rarely well defined, as potential temperature usually has a sloping profile with height at the top of the mixed layer.
- ▶ Long-range transport: consensus was that is still an open question.

Workshop facilitator Bill Petersen asked if any other issues needed discussion before adjournment.

Hearing no response, the Workshop was adjourned early at 11:50 a.m.

7. ACKNOWLEDGMENTS

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APPENDIX A: Executive Summary

Workshop on OB/OD Dispersion Modeling and Atmospheric Measurement Needs

February 15-16, 1995

Boulder, Colorado

SERDP Project 94-251

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1. Introduction

The demilitarization of the U. S. Armed Forces has led to an increase in the stockpile of warfare materials (e.g., munitions, rocket propellants, manufacturing wastes). The current inventory is estimated to be 400,000 tons and growing rapidly at a rate of 40,000 tons per year. The stockpile is distributed throughout the country at more than 200 Department of Defense (DOD) and Department of Energy (DOE) installations. Many of the materials in the stockpile are old, unstable, and unsafe.

Several methods can be employed for the destruction of the stockpile. Incineration, which is commonly used for the disposal of many wastes, is effective for destroying only a small percentage of the material. Chemical treatment techniques are not very effective since they are very costly and only destroy small quantities at a time. The most common disposal method in use today is open burning (OB) and open detonation (OD). OB/OD activities are a relatively simple and cost-effective means for stockpile reduction. However, these activities can generate air pollutants. Any facility that intends to use OB/OD disposal methods must meet permit requirements under subpart X of Part 264 of the Resource Conservation and Recovery Act (RCRA). Source characterization (e.g., rate of plume rise, quantity and identity of pollutants released), meteorological characterization, and atmospheric dispersion modeling are needed to predict the impact of OB/OD emissions on human health and surrounding ecosystems. An OB/OD permit can be issued by an Environmental Protection Agency (EPA) regional office only if the impact is negligible. The problem, however, is that no recommended modeling approach exists; therefore few EPA permits have been granted.

The Strategic Environmental Research and Development Program (SERDP) has funded EPA to develop an OB/OD air pollution dispersion model and mobile meteorological observing platform that will be used to acquire the necessary data for obtaining a RCRA permit. EPA has tasked NOAA's Environmental Technology Laboratory (ETL) to formulate a straw man workplan on the development of a model and monitoring system (included with this document). Recently, a Workshop was held to discuss the design of this system. This Executive Summary briefly outlines the Workshop proceedings and recommendations.

2. Workshop

A Workshop on OB/OD atmospheric dispersion modeling and monitoring was conducted in Boulder, Colorado on February 15 and 16, 1995. The Workshop was hosted by Dr. Robert Banta of ETL and included 26 experts in atmospheric dispersion modeling, surface and upper-air measurements, source characterization and EPA permitting (see Appendix D for a list of these participants and their affiliations). Mr. William Petersen acted as facilitator for the two-day meeting, whose purpose was to present and discuss the strengths and weaknesses of the straw man plan for an OB/OD atmospheric modeling and monitoring system. Major topics of discussion included regulatory permitting requirements, short- and long-range dispersion models of OB/OD plumes, source characterization of the OB/OD, the mobile meteorological measurement platform, and model and measurement platform evaluation and testing.

Regulatory permitting procedures were discussed for OB/OD activities. In general, a facility seeking to obtain a permit submits an application containing information about the type and quantity of the material to be destroyed, the meteorological conditions under which OB/OD would be done, the number of OB/OD activities that will be done annually, the frequency of the OB/OD activities, and how the pollutants and noise released will disperse in the environment. The permit application, which is subjected to careful review, must demonstrate that human health and surrounding ecosystems will not be significantly impacted by the OB/OD activities. . The final determination is made by EPA or by the States in which EPA has delegated its authority.

Short- and long-range transport and dispersion modeling was extensively discussed. The models proposed include a Gaussian puff and a Lagrangian particle model. The problems of complex terrain and model domain were a recurring theme in all discussions. Laboratory simulations in convective tanks would help in parameterization of the plume created from an OB/OD. Valuable information may also be obtained from current OB/OD activities. Regardless of the type of model to be used, a minimum amount of information will be needed for model input. This includes mixed layer height, boundary layer winds and temperature structure, cloud size and temperature, mass of material to be destroyed and its chemical content, and surface momentum and heat fluxes. Questions of plume penetration of the elevated inversion layers and transport into the free atmosphere was another recurring theme. Long-range transport can occur as a result of plume penetration. Generally this is undesirable because of perceived permitting problems for significant off-site impacts.

Critical to the success of the transport and dispersion model will be the accurate characterization of the OB/OD source. Needed information includes the heat released during an OB/OD, plume expansion and rise, amount of dust entrained into an OD plume, contents of the munitions being destroyed, chemical reactions of those contents during an OB/OD, particle size distribution, possible interactions of those particulates with other atmospheric aerosols. Access to this information, will ensure an accurate assessment of the impact air pollutants will have on ecosystems downwind of an OB/OD.

The proposed design for the mobile meteorological platform met with approval. The system will include a 915-MHz, wind-profiling radar to obtain horizontal and vertical wind profiles from heights of 100 m above ground up to 3,000 m over 100 m intervals; a radio acoustic sounding system (RASS) for the acquisition of virtual air temperature profiles from 100 m up to 1,500 m over 100 m intervals; an acoustic sodar system to obtain high-resolution (25-m) horizontal and vertical wind profiles in the first 500 m of the boundary layer; a mini-lidar system to estimate mixed layer height; and at least one 10-m tower system to obtain surface layer measurements of wind speed and direction, air temperature, relative humidity, solar radiation, barometric pressure, and turbulence variables such as fluxes of sensible heat and momentum. These instruments will be "off-the-shelf" technology that will be integrated with a workstation in a modular fashion, allowing for future integration of more sensing devices if the need arises. All data from these systems will be fed into a workstation for numerical model simulations.

Discussions included the design and implementation of extensive testing of the model and measurement platform. Initial shakedown of the monitoring system would be conducted at the Boulder Atmospheric Observatory, where a 300-m tower would allow for side-by-side comparison of the data obtained from the profiling systems. Eventually, the monitoring system (along with the dispersion model) would be transported to various DOD and DOE facilities for evaluation. However, no specific facilities were chosen at the Workshop, and development of more detailed work plans for field testing were recommended.

3. Recommendations and Conclusions

Workshop members experienced with the EPA permitting process stated that obtaining an EPA permit would be difficult for OB/OD activities having an environmental impact extending beyond 30 km. This could limit the total mass of materials to be destroyed and the atmospheric conditions under which OB/OD activities could be conducted. A special emphasis was placed on the development of more detailed source characterization. This includes information on the pollutants released, initial plume or puff size and rise, and size distribution of dust particles entrained into an OB/OD. Complex topography was another issue of concern. Since many depots are located in mountainous terrain, establishment of a representative wind field may be difficult if using only one wind profiling system in one location. The use of multiple 10-m towers may help establish a representative wind field for the dispersion model.

Extensive field testing of the model and mobile meteorological observing system was also recommended, preferably at several facilities with various topographies and atmospheric conditions. This would help to establish the overall performance of the model and monitoring system.

A central point of contact for this project was recommended. Gennaro Crescenti will act as the EPA program manager and be the liaison between all of the project components. He will periodically send out updates on program status to all Workshop participants and help coordinate project activities.

APPENDIX B:

**ATMOSPHERIC DISPERSION MODEL DEVELOPMENT
FOR OPEN BURN/OPEN DETONATION EMISSIONS**

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INTRODUCTION

The disposal of the demilitarization stockpile—unwanted munitions, rocket propellants, and manufacturing wastes—is necessary at Department of Defense (DOD) and Department of Energy (DOE) installations. The disposal methodologies include: 1) recovery and reclamation technology, 2) thermal destruction methods such as incineration and popping furnaces, 3) research stage technology such as electrochemical reduction and biodegradation, and 4) open burning (OB) or open detonation (OD) (Ref. 1). OB/OD takes place in an earthen pit, trench, or bermed area and is the most common disposal method in use today; this stems from its low cost, effectiveness, and the capacity to treat a wide range of munitions.

The existing demilitarization stockpile is estimated to be about 400,000 tons and is increasing at the rate of about 40,000 tons per year.² However, the material destroyed in a single detonation typically ranges only from 100 to 5000 lbs, while the quantity treated in a burn is somewhat larger and usually lasts from 1 to 5 min. Thus, a large number of detonations or burns will be required to significantly reduce the existing stockpile.

OB/OD operations generate air pollutants and require predictions of pollutant concentrations to assess air quality impacts and health risks. The pollutants include SO_2 , NO_x , CO, particulates, volatile organic compounds and hazardous or toxic materials such as metals, cyanides, semivolatile organics, etc.^{2,3} For very large detonations ($1 - 3 \times 10^4$ lbs), natural dust entrained by the blast is an additional contaminant to consider. Emissions from OB/OD sources have the following special features: 1) "instantaneous" or short-duration releases of buoyant material, 2) considerable variability in the initial cloud size, shape, and height, and 3) ambient exposure times for individual clouds that are significantly less than the typical averaging times (≥ 1 hr) of air quality standards.

Predictions of air quality impact require the use of atmospheric dispersion models together with model inputs on source and meteorological conditions. Currently, there is no recommended EPA model to handle the special features of OB/OD sources. The most commonly-used approach is INPUFF,^{4,5} a Gaussian puff model. The basic puff framework is suitable for OB/OD releases although the existing INPUFF has several limitations as discussed below. As a result, a model development program was initiated under the sponsorship of the DOD/DOE Strategic Environmental Research Development Program.

In the following, we discuss: 1) background issues influencing the development of an OB/OD dispersion model, 2) a model development overview, and 3) the framework for short-range modeling (distances $\lesssim 30$ km). Plans for long-range modeling (distances $\gtrsim 30$ km) are in the initial stages of development and will be described later. The model development program began in September 1994 along with a parallel effort to construct a mobile meteorological platform, which is necessary due to the remoteness of many of the DOD facilities. A related program has been acquiring information on OB/OD emission factors from experimental test chambers³ and field studies.²

BACKGROUND

Several factors have motivated and influenced the development of an OB/OD dispersion model including: 1) the limitations of existing models, 2) the improved knowledge of the planetary boundary layer (PBL), 3) potential future OB/OD operations, and 4) the development of a mobile meteorological platform. These topics are briefly discussed in the following.

Limitations of Existing Models

As noted earlier, the INPUFF Model^{4,5} is a commonly-used approach for dealing with OB/OD sources and can handle dispersion from individual puffs or clouds or from a sequence of puffs as in a short-duration release, e.g., an open burn. Although the Gaussian puff approach is appropriate for OB/OD sources, INPUFF has the following limitations:

- 1) It uses dispersion parameters (σ_y, σ_z) from the Pasquill-Gifford (PG) curves⁶, which are only applicable to surface releases, or from Irwin's scheme.⁷
- 2) It adopts Briggs' plume rise expressions⁸ which apply to continuous releases rather than to instantaneous sources (puffs, clouds, or thermals) and does not address buoyant thermal penetration of elevated inversions capping the PBL. Thermal penetration of the inversion may be important for large detonations or burns.
- 3) It assumes Gaussian statistics for turbulent lateral and vertical velocities in the PBL, whereas the vertical velocity statistics in the unstable PBL are positively skewed.⁹ The skewness should be included for vertical dispersion.¹⁰
- 4) It does not address transport and dispersion in the vicinity of shorelines, mountains, and other complex terrain.

From a scientific viewpoint, use of the PG curves is deficient in that 1) they are based on dispersion from a ground-level source and for short downwind distances (< 1 km) and 2) the curve selection scheme is based on surface meteorology, which does not account for the vertical structure of PBL turbulence.¹⁰ For large detonations or burns, source buoyancy can carry emissions to several hundred meters or to the top of the PBL, with the possible penetration of the capping inversion. One must then deal with dispersion throughout the entire PBL and have a better characterization of buoyancy effects.

Other dispersion models for OB/OD sources have been proposed and are described in Ref. 11.

Turbulence and Dispersion in the Planetary Boundary Layer

Over the past two decades, much progress has occurred in our knowledge of turbulence and dispersion in the PBL,¹² both for the unstable or convective boundary layer (CBL) and the stable boundary layer (SBL). For the CBL, numerical and laboratory simulations and field observations revealed the large-scale flow structures and the

important turbulence velocity and length scales—the convective velocity scale w_* and the CBL height h . Typical values of w_* and h at midday are 1 - 2 m/s and 1500 m. Major insights into dispersion followed from laboratory experiments, numerical simulations, and field observations for both nonbuoyant and buoyant plumes.^{10,13,14}

For the SBL, the turbulence is much weaker with typical eddy sizes on the order of tens of meters or less.⁹ Numerical models and field observations have demonstrated that wind shear is the important source of turbulence with the friction velocity u_* being the relevant velocity scale; u_* is typically of the order of 0.1 m/s in strongly stable conditions. Dispersion has been put into a sound framework for near-surface sources, whereas the framework is less general for elevated releases.¹⁵ Nevertheless, models have led to a good understanding and organization of observations.

The application of the improved knowledge of the PBL has been discussed in a number of short courses and monographs and is now being incorporated into models for applications.¹² A recent example is AERMOD¹⁶ for industrial source complexes. Knowledge of flows, dispersion, and other processes over complex terrain is summarized in another recent monograph.¹⁷

Potential Future OB/OD Operations

In contemplating a significant reduction of the demilitarization stockpile, consideration is being given to much larger detonations (e.g., 1 - 5 × 10⁴ lbs) than those currently used because of the higher temperatures and more efficient thermal destruction of contaminants. Possible dispersion scenarios include: 1) a large daytime release with sufficient source buoyancy to carry material to the top of the CBL with possible penetration of the elevated inversion, and 2) a large nighttime release with sufficient buoyancy to carry the emissions above the SBL into the overlying weakly- or non-turbulent airflow. In both scenarios, the source material could be transported large distances (~ 20 to 100 km) with significant lateral dispersion but minimal vertical dispersion, thus preventing high ground-level concentrations (GLCs) near the source. The avoidance of a high near-source impact would increase the importance of long-range transport with somewhat lower GLCs.

Mobile Meteorological Platform

Due to the remoteness of many DOD facilities, a mobile meteorological platform is being developed to provide the PBL variables necessary for modeling. The initial platform design contains: 1) a radar wind profiler for obtaining profiles of the three wind components to a height of 3 km, 2) a radio acoustic sounding system (RASS) for temperature profile measurements, 3) a mini-SODAR for measuring profiles of wind and the vertical turbulence component (σ_w) to a height of ~ 200 m, 4) a mini-lidar system for measuring the PBL depth, and 5) a portable meteorological station for measuring near-surface winds, temperature, turbulence, and heat flux. The dispersion model should be designed to maximize the use of the data from this platform, with the temporal and spatial resolution of the measurements being determined by instrument limitations and modeling needs.

MODEL DESIGN OVERVIEW

In the following, we give a brief overview of the key features to be included in the OB/OD dispersion model and the division by model types. The important features to address in the modeling are:

- 1) all aspects of the source including the instantaneous nature of the release, the cloud or thermal rise, thermal penetration of an elevated inversion, and the short exposure time of the cloud,
- 2) modern dispersion concepts¹² based on the turbulence structure and scaling of the CBL and SBL,
- 3) use of micrometeorological variables along with vertical profiles of wind, temperature, and turbulence from the mobile meteorological platform,
- 4) short- and long-range dispersion where the distinction between them is taken at a distance of ~ 20 to 30 km, and
- 5) a treatment of complex terrain which exists in the vicinity of many DOD facilities in the western US.

In addition, the design should consider: 1) modeling of the dose (time integral of the concentration) as well as the concentration with provisions for determining the time-averaged concentration that is necessary in air quality assessments, and 2) short-term fluctuations in concentration and dose, and 3) deposition of particles.

The modeling is divided in two ways: 1) short- and long-range dispersion, and 2) modeling methodology which refers to the degree of detail, spatial resolution, and computation. The division at a scale of 20 to 30 km is somewhat arbitrary but intended to distinguish a regime where simple wind field modeling may be accomplished (short range) and one where a more complete wind field model is necessary (long range), i.e., for transport times exceeding ~ 1 hr. Ultimately, the short-range model would be a component of or treated as an initial "subgrid" approach in the long-range model.

The modeling methodology is divided into an applications approach with relatively low computational costs and a research model. For the applications methodology, a Gaussian puff model is proposed whereas a Lagrangian particle model is planned for the research approach. The applications model would be useful for routine problems in regulatory permitting, whereas the research model is necessary to address more complicated issues, e.g., inversion penetration, complex terrain, and those associated with larger detonations.

SHORT-RANGE MODEL

Applications Model

The following pertains to the model for an instantaneous release or detonation. The concentration field for an open burn or short-duration release is obtained by integrating the concentration expression for the instantaneous source or puff over time, i.e., integrating the concentration over a sequence of puffs from successive release times. This is briefly discussed under cloud rise below.

Concentration field. Dispersion models predict the ensemble-mean concentration C for a given set of source and meteorological conditions, i.e., the concentration that would be observed if the same experiment—same source and meteorological conditions—were repeated a large number of times. For now, our focus is on the C for a given averaging time, but it should also be possible to model the rms concentration fluctuation (e.g., see Ref. 18). In this section, we discuss near-instantaneous or short-term concentrations; time-averaged concentrations are considered under the dosage.

Currently, it is not clear what short-term concentrations are relevant for permitting situations and we consider two estimates: the peak and the mean at a downwind location. Both are obtained from a Gaussian puff model for C (see Ref. 19):

$$C = \frac{Q}{(2\pi)^{3/2} \sigma_{rx} \sigma_{ry} \sigma_{rz}} \exp \left[-\frac{(x - Ut)^2}{2\sigma_{rx}^2} - \frac{y^2}{2\sigma_{ry}^2} - \frac{(z - h_e)^2}{2\sigma_{rz}^2} \right], \quad (1)$$

where Q is the pollutant mass released, U is the mean wind speed, t is the travel time, h_e is the effective puff or cloud height, and σ_{rx} , σ_{ry} , and σ_{rz} are the puff standard deviations in the x , y , and z directions, respectively. Here, $h_e = h_s + \Delta h$ where h_s is the source height and Δh is the cloud rise due to buoyancy, x is the distance in the mean wind direction, y is the crosswind distance, and z is the height above ground. Equation (1) describes the concentration field relative to the puff centroid.

Peak concentration. The peak concentration is that in the elevated buoyant puff which could be carried to the surface by a strong downdraft in the PBL, especially in the CBL. The puff centroid concentration C_c is

$$C_c = \frac{Q}{(2\pi)^{3/2} \sigma_{rx} \sigma_{ry} \sigma_{rz}}. \quad (2)$$

For simplicity, the puff can be considered to be isotropic: $\sigma_{rx} = \sigma_{ry} = \sigma_{rz} = \sigma_r$. For a buoyant puff, σ_r is proportional to the puff radius as discussed below.

If C_c is used as an estimate of the peak surface concentration, an estimate should be given of its probability of occurrence there. One possible way of doing this is to consider random puff trajectories due to the random vertical velocity w in the PBL:

$$z_p = h_s + \frac{wx}{U} + \Delta h(x), \quad (3)$$

where z_p is the random puff height. The probability $P(z \leq z_\ell)$ that the centroid could be carried to the surface is found from

$$P(z \leq z_p) = \int_0^{z_\ell} p(z_p) dz_p, \quad (4)$$

where $p(z_p)$ is the probability density function (p.d.f.) of z_p and z_ℓ is a small height near the surface, e.g., $z_\ell \simeq \sigma_r/2$. The $p(z_p)$ can be found from the p.d.f. of w [$p_w(w)$] according to¹⁰

$$p(z_p) = p[w(z_p); x] \left| \frac{dw}{dz_p} \right|, \quad (5)$$

where w and dw/dz_p are found from Eq. (3).

Mean concentration. The mean concentration at a given height due to all of the random updrafts and downdrafts is given by Eq. (1) but with the σ_{rz} replaced by σ_z , which corresponds to the absolute dispersion (i.e., from Taylor's theory, Eq. 17 below). This mean concentration is relevant for the SBL or in the limit of a neutral boundary layer where a Gaussian w p.d.f. is applicable. However, for the CBL, a positively-skewed w p.d.f. is more consistent with laboratory and field data and should be adopted.

For the CBL, a good approximation to the w p.d.f. (p_w) has been shown to be the superposition of two Gaussian distributions¹⁰

$$p_w = \frac{\lambda_1}{\sqrt{2\pi}\sigma_1} \exp\left(-\frac{(w - \bar{w}_1)^2}{2\sigma_1^2}\right) + \frac{\lambda_2}{\sqrt{2\pi}\sigma_2} \exp\left(-\frac{(w - \bar{w}_2)^2}{2\sigma_2^2}\right), \quad (6)$$

where λ_1 and λ_2 are weighting coefficients for the distributions with $\lambda_1 + \lambda_2 = 1$. The \bar{w}_j and σ_j ($j = 1, 2$) are the mean vertical velocity and standard deviation for each distribution and are assumed to be proportional to σ_w . The $\bar{w}_1, \bar{w}_2, \sigma_1, \sigma_2, \lambda_1, \lambda_2$ are found as a function of σ_w , the vertical velocity skewness $S = \bar{w}^3/\sigma_w^3$ where \bar{w}^3 is the third moment of w , and a parameter $R = \sigma_1/\bar{w}_1 = -\sigma_2/\bar{w}_2$ (Ref. 20). This requires σ_w^2 , which is parameterized in terms of w_* and the friction velocity u_* (see Ref. 10), and \bar{w}^3 which is taken as $\bar{w}^3 = 0.125w_*^3$ in the upper 90% of the CBL.

The vertical concentration distribution is derived from p_w following the same approach as applied to continuous plumes.¹⁰ The resulting expression for C is given by

$$C = \frac{Q}{(2\pi)^{3/2} \sigma_{rx} \sigma_{ry}} \exp\left(-\frac{(x - Ut)^2}{2\sigma_{rx}^2} - \frac{y^2}{2\sigma_{ry}^2}\right) \times \left[\frac{\lambda_1}{\sigma_{z1}} \exp\left(-\frac{(z - h_e - \bar{z}_1)^2}{2\sigma_{z1}^2}\right) + \frac{\lambda_2}{\sigma_{z2}} \exp\left(-\frac{(z - h_e - \bar{z}_2)^2}{2\sigma_{z2}^2}\right) \right], \quad (7)$$

where

$$\sigma_{zj} = \frac{\sigma_j x}{U} \quad \text{and} \quad \bar{z}_j = \frac{\bar{w}_j x}{U} \quad \text{with } j = 1, 2. \quad (8)$$

The λ_j , σ_j , and $\overline{w_j}$ ($j = 1, 2$) are the parameters appearing in Eq. (6). Equation (7) applies only for small x such that the plume interaction with the ground or elevated inversion is weak.

More complete expressions for C corresponding to (4) are applicable in the case of multiple cloud reflections at the ground and PBL top.

Dosage. There are practical advantages in modeling the dosage when analyzing the air quality impact due to instantaneous sources. The partial dosage ψ is defined by

$$\psi(x, y, z, t) = \int_0^t C(x, y, z, t') dt' \quad (9)$$

and the total dosage by $\psi_\infty = \psi(x, y, z, \infty)$. One advantage is that ψ should be a more stable statistic than the concentration due to the time integration, and this has value in the analysis of field data and model evaluation. Second, the time-averaged concentration over 1 hr periods or longer is necessary.

For clouds with short passage times over a receptor, the average concentration \overline{C} can be obtained from

$$\overline{C} = \frac{\psi(t_2) - \psi(t_1)}{T_a}, \quad (10)$$

where the averaging time $T_a = t_2 - t_1$. The puff passage time is $\sim 4\sigma_{rz}/U$ and if this is less than T_a , then $\overline{C} = \psi_\infty/T_a$.

The integration in Eq. (9) can be carried out analytically for limiting forms of the σ_{rx} , σ_{ry} , σ_{rz} , and Δh variation with t . For example, this can be done for $\Delta h = 0$ and $\sigma_{rx}, \sigma_{ry}, \sigma_{rz} \propto t$ or $\propto t^{1/2}$. These and other forms or combinations of them must be examined to determine which of the physically meaningful cases result in an analytical integration in (9). Otherwise, a numerical integration of Eq. (9) is necessary.

If it is assumed that σ_{ry} and σ_z are constant during the puff passage time over a receptor (i.e., the passage time is short), then

$$\psi_\infty = \frac{Q}{2\pi U \sigma_{ry} \sigma_z} \exp \left(-\frac{y^2}{2\sigma_{ry}^2} - \frac{(z - h_s)^2}{2\sigma_z^2} \right) \quad (11)$$

as pointed out by Gifford.¹⁹ Equation (11) is of the same form as the expression for C due to a continuous point source, but here Q is the total contaminant mass and not the release rate.

Cloud rise and inversion penetration. For neutral air, the governing equations for puffs or thermals give the thermal rise as a function of time and the initial momentum and buoyancy, but experiments must be conducted to determine an entrainment coefficient (see Refs. 21, 22, 23). From a combination of theory and laboratory experiments, Scorer²² obtained the following expression for the rise

$$\Delta h = 2.35(M_T t + F_T t^2)^{1/4}, \quad (12)$$

where M_T and F_T are the initial momentum and buoyancy of the thermal. They are given by

$$M_T = \frac{4\pi}{3} r_o^3 w_o \quad \text{and} \quad F_T = \frac{g Q_T}{c_p \rho_a T_a}, \quad (13)$$

where w_o , r_o , and Q_T are the initial velocity, radius, and heat content of the thermal, g is the gravitational acceleration, c_p is the specific heat of air, and ρ_a and T_a are the ambient air density and temperature.

Scorer also reported that the puff radius r was on average given by $r = 0.25 \Delta h_t$, where Δh_t is the cloud top height. However, there was considerable variability in the above coefficient which ranged from 0.14 to 0.5. The relative dispersion $\sigma_r \propto r$.

Using field observations from small munitions and larger detonations, Weil²⁴ confirmed that Eq. (12) was a good fit to data over a wide range of times following the release. Thus, Eq. (12) is suitable for the initial rise of a cloud, i.e., before it is limited by stable stratification. The initial heat content Q_T of the cloud can be determined from the mass of the detonation using the conversion 1100 kcal/kg TNT (see Church²⁵).

In stable air, the maximum cloud rise was found by Morton et al.²³ to be

$$\Delta h = 2.66 \frac{F_T^{1/4}}{N^{1/2}}, \quad (14)$$

where N is the Brunt-Vaisalla frequency; $N^2 = (g/\Theta)(\partial\Theta/\partial z)$ where Θ is the ambient potential temperature.

For thermal or cloud penetration of an elevated density jump, results have been obtained from laboratory experiments in a nonturbulent environment. Saunders²⁶ derived the cloud height history and maximum penetration height as a function of F_T , the density jump $\Delta\rho_i$, and its height. Richards²⁷ obtained an empirical expression for the fraction P of the cloud penetrating the jump:

$$P \simeq 1 - 0.5 \frac{\Delta\rho_i}{\Delta\rho_{Ti}}, \quad (15)$$

where $\Delta\rho_{Ti}$ is the average density excess of the cloud when it reaches the density jump. The $\Delta\rho_{Ti}$ can be estimated from F_T and the cloud radius (r) growth law, $r \propto \Delta h$.

Initial criteria for the cloud fraction $1 - P$ trapped below a thin inversion can be developed from the above results. This can then be used in the dispersion model. However, the problem should be pursued further to: 1) develop consistency between the approach used for clouds or thermals and those used for plumes (e.g., Briggs,²⁸ Manins,²⁹ and Weil³⁰), 2) extend the model for P to a thick elevated inversion characterized by the $\partial\Theta/\partial z$, and 3) conduct further laboratory experiments on thermal penetration of density jumps and thick inversions. The latter experiments should be conducted in both the presence and absence of convective turbulence below the inversion.

Dispersion parameters. Puff or relative dispersion. For detonations (instantaneous sources), the puff growth is initially dominated by buoyancy-induced entrainment and r follows $r \propto \Delta h \propto t^{1/2}$ as given above. The puff should also grow due to the ambient turbulence in the inertial subrange although the observational base for this (in the case of buoyant sources) is not well defined. Based on modeling for plumes,^{8,31} a tentative expression for the puff or cloud radius growth is

$$\frac{dr}{dt} = \alpha_1 w_p + \alpha_2 v_e, \quad (16)$$

where w_p is the puff rise velocity, $v_e = (2\epsilon r)^{1/3}$ is an inertial-range velocity, ϵ is the ambient turbulent energy dissipation rate, and α_1, α_2 are empirical entrainment coefficients. Equation (16) represents a simple superposition of the entrainment due to buoyancy-induced turbulence and ambient inertial-range turbulence.

The analogous expression (to 16) for plumes was used recently to model the mean and rms fluctuating concentrations due to a buoyant plume in the CBL. The approach produced fair agreement with the Deardorff and Willis laboratory measurements in a convection tank.³²

Equation (16) is a first attempt at a difficult problem and one where laboratory and field data would be invaluable. In particular, convection tank measurements of buoyant puff dispersion and concentration fields would be very beneficial to the modeling program.

Absolute dispersion. For a sufficiently long-duration burn (to be defined), the "instantaneous" or short-time averaged concentration could be determined from a plume model (Gaussian or p.d.f. approach) with absolute dispersion for σ_z (Eq. 17) and relative dispersion (σ_{ry}) for the lateral component. However, longer time averages (say > several minutes) can be determined using absolute or plume dispersion parameters for both the y and z components. The lateral (σ_y) and vertical (σ_z) plume standard deviations can be found from a parameterization of Taylor's statistical theory:¹⁵

$$\sigma_y = \frac{\sigma_v t}{(1 + t/2T_{Ly})^{1/2}}, \quad \sigma_z = \frac{\sigma_w t}{(1 + t/2T_{Lz})^{1/2}}, \quad (17)$$

where T_{Ly}, T_{Lz} are the Lagrangian time scales for the v and w components and $t = x/U$.

The time scales can be parameterized using expressions such as $T_{Lz} \propto \sigma_w/h$, $T_{Lz} \propto \sigma_w^2/\epsilon$, etc. as done previously.^{14,15,20} The PBL variables necessary in these and other expressions— $\sigma_u, \sigma_v, \sigma_w, \epsilon$, surface fluxes, etc.—would be obtained from the meteorological platform.

Complex terrain. The treatment of dispersion in hilly or complex terrain will vary depending on the wind field input. In the case of wind profile measurements only (no diagnostic or prognostic modeling), the dispersion model focus would be on the cloud impaction about the windward side of a hill. The approach would be similar to that used in the EPA CTDMPLUS model^{33,34} or a simpler method.¹⁶ This accounts for flow

speedup over a hill, plume deformation, turbulence changes, and their effects on the surface concentration through a modification to the Gaussian plume model. In addition, it accounts for the concept of a dividing streamline height (H_c) in stably-stratified flow, where ambient air tends to travel around a hill for $z < H_c$ and over the hill for $z > H_c$. This approach accounts for dispersion about the first hill downwind of a source and has obvious limitations for sources in complex terrain consisting of many ridges, hills, and valleys.

Wind field. There are three general categories of wind field input to the puff model that are being considered. As noted below, these would be used differently.

1. Observed vertical profiles of the time-varying wind at a single (x, y) location. These are obtained from the mobile meteorological platform. For modeling, the observed winds would be considered representative of the wind field over some short range (perhaps 10 to 20 km or so); obviously, this depends on the terrain. The puff displacements would be tracked using the wind components for each sequential time interval. This would be used in the most routine applications and for assessing air quality impact with historical meteorological data as input.
2. Diagnostic wind model. This approach uses observed winds over an x, y domain (mobile platform and other data) coupled with the continuity equation and an interpolation scheme to obtain a mass-consistent wind field (e.g., Ref. 35). This could only be practicable at sites where adequate wind measurements (a grid) are available and probably only for selected meteorological scenarios; e.g., this would not be used with historical wind data for every hour of the year. This approach has particular limitations in complex terrain and for stably-stratified flow.
3. Prognostic wind model. This approach³⁶ could be used for selected meteorological scenarios with observed winds from the mobile platform and other sources as input. When used with four dimensional data assimilation (e.g., Refs. 37 and 38), this could be the most general approach for obtaining the wind field. Key limitations are the computational resources necessary and the grid resolution.

Turbulence field. The profiles of $\sigma_u, \sigma_v, \sigma_w$ would be obtained from combined use of the observed σ_w profiles (lowest 200 m), the $\sigma_u, \sigma_v, \sigma_w$ surface observations, surface heat and momentum flux measurements, and parameterizations of the turbulence variables at other sites (similarity profiles, e.g., see Refs. 9, 10, 15). The parameterizations would be used for guidance as site-specific turbulence profiles may be generated; a parameterization of ϵ also would be needed. In addition, the PBL depth would be obtained from the mini-lidar.

Other effects. The applications model also will contain descriptions and expressions for dealing with dust generated by the cloud, deposition of particles (e.g., Ref. 39), and possibly concentration fluctuations.

Research Model

A Lagrangian statistical model is being considered for addressing several aspects of short-range dispersion. In this approach,²⁰ one follows "particles" in a turbulent flow given 1) the Eulerian velocity statistics, or 2) the time-dependent Eulerian velocity fields; the latter are obtained from large-eddy simulations (LES) of the PBL. Currently, the Lagrangian approach is being used to model the fluctuating as well as the mean concentration field due to a passive scalar source in the CBL, using LES-generated velocity fields.

The dispersion of buoyant plumes has been computed using a hybrid Lagrangian model that relies on parameterized profiles of the Eulerian velocity statistics.³² This deals with both the fluctuating and mean concentration distributions. The modeling can be extended to: 1) treat buoyant puffs, and 2) use the LES fields as input rather than the parameterized turbulence.

MODEL EVALUATION

At present, the OB/OD dispersion model development includes plans for testing the model with three types of data bases.

- 1) Laboratory data. As noted earlier, laboratory experiments on cloud or thermal penetration of elevated inversions would be useful for model testing. We plan to conduct such experiments in a salt-stratified tank in the absence of any ambient or background turbulence. The experiments would be similar to those conducted by Saunders²⁶ and Richards²⁷ with turbulent thermals except that we will include a constant density stratification above a neutral layer in addition to a density jump above the neutral layer. In addition, it is planned to test ambient turbulent dispersion aspects of the model using instantaneous releases in a laboratory convection tank. The experiments are planned for the EPA Fluid Modeling Facility in Research Triangle Park, NC.
- 2) Existing field data. A survey of existing data bases on the rise of buoyant clouds and short-duration plumes from surface releases will be made. It is anticipated that such data exist at military installations with that used by Weil²⁴ from the White Sands Missile Range as an example. The latter included cloud rise from detonations as well as a plume from an oil fire. These data would be used to test the initial buoyant rise phase of clouds and plumes in the PBL.
- 3) Future field experiments. Currently, it is planned to conduct future field experiments on the rise and dispersion of buoyant clouds and plumes from OB/OD sources. In addition to detailed meteorological data from towers and the mobile platform, we will track and measure the dispersion of the airborne clouds and plumes with a lidar, i.e., to obtain the cloud geometry. We also will consider ambient concentration measurements of cloud constituents with the feasibility of such measurements determined by model calculations and instrument capabilities.

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APPENDIX C:

12.5 DISPERSION MODEL DEVELOPMENT FOR OPEN BURN/OPEN DETONATION SOURCES

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1. INTRODUCTION

The disposal of obsolete munitions, propellants, and manufacturing wastes is conducted at Department of Defense (DOD) and Department of Energy (DOE) facilities. The most common disposal method is open burning (OB) and open detonation (OD) of the material, which occurs in an earthen pit or bermed area. At present, the material destroyed in a single detonation typically ranges from 100 to 5000 lbs, whereas the quantity treated in a burn can be somewhat larger and last from minutes to an hour. OB/OD activities are restricted to daytime during unstable or near-neutral atmospheric stability.

OB/OD operations generate air pollutants and require predictions of pollutant concentrations. The pollutants include SO_2 , NO_x , particulates, volatile organic compounds and toxic materials such as metals, semivolatile organics, etc. (Andrulis, 1992). For large detonations ($1 - 3 \times 10^4$ lbs), natural dust entrained by the blast is an additional contaminant. Emissions from OB/OD sources have the following unique features: 1) "instantaneous" or short-duration releases of buoyant material, 2) a wide variability in the initial cloud size, shape, and height, and 3) ambient exposure times from clouds that are much less than the typical averaging times (~ 1 hr) of air quality standards.

Dispersion models are used to estimate pollutant concentrations given the source and meteorological conditions. However, there is currently no recommended EPA dispersion model to address

OB/OD sources. The most widely-used approach is INPUFF (Petersen, 1986), a Gaussian puff model, but this has several limitations as discussed below. Due to the constraints of existing models, a model development program was initiated under the DOD/DOE Strategic Environmental Research and Development Program.

In Section 2, we give an overview of the model design which is divided into "simple" and "research" components. Sections 3 and 4 describe the simple component which includes Gaussian puff and analytic plume models. This development program is in progress and is currently limited to the unstable planetary boundary layer (PBL).

2. MODEL DESIGN CONSIDERATIONS

2.1 Background

The development of an OB/OD dispersion model has considered: 1) the limitations of existing models, 2) current knowledge of turbulence and dispersion in the PBL, and 3) a mobile meteorological platform under development.

Limitations of existing models. INPUFF has been used to model OB/OD sources and can handle dispersion from individual puffs or clouds or from a sequence of puffs in a short-duration release. Although the Gaussian puff approach is suitable for OB/OD sources, INPUFF has the following limitations: 1) It adopts dispersion parameters (σ_y, σ_z) from the Pasquill-Gifford (PG) curves or from Irwin's (1983) scheme. 2) It includes Briggs' (1971) plume rise expressions which apply to continuous releases rather than to instantaneous sources (puffs, clouds) and does not address thermal penetration of elevated inversions capping the PBL. 3) It assumes Gaussian velocity statistics for the turbu-

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lence, whereas the vertical velocity statistics in the unstable PBL are positively skewed (Wyngaard, 1988). The skewness should be included for vertical dispersion.

For OB/OD sources, the PG curves are deficient in that they: 1) are based on dispersion from a ground-level source and short downwind distances (< 1 km), and 2) are selected using surface meteorology, which does not account for the PBL's vertical structure. For large detonations, source buoyancy can carry emissions to several 100 m or the PBL top; one must then deal with dispersion over the entire PBL.

PBL turbulence. Dispersion in the PBL depends on the turbulence length and velocity scales which differ for the unstable or convective boundary layer (CBL) and the stable boundary layer (SBL). For the CBL, the length and velocity scales are the CBL depth h and the convective velocity scale w_* . Typical values of w_* and h at midday over land are 1 - 2 m/s and 1 - 2 km. Within the "mixed layer" ($0.1h \leq z < h$), the mean wind speed and turbulence components—longitudinal σ_u , lateral σ_v , and vertical σ_w —vary little with height z ; in strong convection, $\sigma_u, \sigma_v, \sigma_w \approx 0.6w_*$.

For the SBL, the turbulence is much weaker with eddy sizes proportional to z near the surface and typically ~ 10 s of meters or less in the upper part of the SBL. Models and observations show that the velocity scale is the friction velocity u_* (Wyngaard, 1988), which is typically ~ 0.1 m/s in strong stable stratification.

Knowledge of the PBL turbulence structure has been included in models for applications (see Venkatram and Wyngaard, 1988).

Mobile meteorological platform. A mobile meteorological platform is being developed at NOAA-ETL to obtain the PBL variables necessary for modeling since many DOD facilities are in remote locations. The platform design includes: 1) a radar wind profiler for obtaining the three wind components up to ~ 3 km, 2) a radio acoustic sounding system (RASS) for temperature measurements, 3) a mini-SODAR for measuring winds and σ_w to a height of ~ 200 m, 4) a mini-lidar system for obtaining the PBL depth h , and 5) a portable meteorological station for measuring near-surface winds, temperature, turbulence, and heat flux. The dispersion model is being designed for efficient use of these measurements.

2.2 Overall Model Design

A model hierarchy is planned including: 1) a simple computational framework for routine problems, and 2) a more detailed or research model for nonroutine problems. In the simple approach, a Gaussian puff model is adopted for instantaneous

sources and puff, integrated-puff, and plume models for short-duration releases. For the research framework, a Lagrangian particle and/or puff approach is planned. Both frameworks will be considered for "onsite" use in a real-time operational mode using data from the mobile meteorological platform, i.e., for day-to-day decisions on OB/OD operations. The puff and plume models would be used for climatological analyses needed in risk assessments.

In modeling, the important aspects to address are: 1) all source-related features including the instantaneous or short-duration nature of the release, buoyancy-induced rise and dispersion, and cloud or plume penetration of elevated inversions, 2) relative and absolute dispersion expressions that explicitly include PBL turbulence variables, 3) meteorological variables including their vertical profiles from the mobile platform, and 4) a treatment for puff and plume dispersion about complex terrain.

The following models address points 1 and 2 above and must be expanded to include points 3 and 4. Further development also will address: 1) a more complete description of initial source effects (detonation cloud size and height) and inversion penetration, 2) a more complete PBL turbulence parameterization, 3) averaging time effects on concentration, 4) the entrained dust source term, and 5) deposition of gases and particles.

3. INSTANTANEOUS SOURCES

3.1 Dispersion Model

Concentration. For instantaneous sources or detonations, a Gaussian puff model is adopted for the short-term mean concentration (C) field:

$$C = \frac{Q}{(2\pi)^{3/2} \sigma_{rx} \sigma_{ry} \sigma_{rz}} \times \exp \left[-\frac{(x - Ut)^2}{2\sigma_{rx}^2} - \frac{y^2}{2\sigma_{ry}^2} - \frac{(z - h_e)^2}{2\sigma_{rz}^2} \right], \quad (1)$$

where Q is the pollutant mass released, U is the mean wind speed, t is the travel time, h_e is the effective puff height, and σ_{rx} , σ_{ry} , and σ_{rz} are the puff standard deviations or relative dispersion in the x , y , and z directions, respectively. Here, $h_e = h_s + \Delta h$ where h_s is the source height and Δh is the cloud rise due to buoyancy; x and y are the distances in the mean wind and crosswind directions.

Currently, we are considering two approaches for estimating the peak ground-level concentration (GLC) at a given x : 1) the peak concentration C_c in the elevated buoyant puff, and 2) a peak found from a probability distribution of concentration at a downwind receptor. The C_c is the puff centroid

concentration given by $C_c = Q/[(2\pi)^{3/2}\sigma_{rx}\sigma_{ry}\sigma_{rz}]$, where the relative dispersion parameters are generally different in the three directions. In the following, we assume $\sigma_{rx} = \sigma_{ry} = \sigma_{rz} = \sigma_r$. If C_c is used as an estimate of the peak concentration, an estimate must be made of the probability of it being brought to the surface: one possible method is given by Weil et al. (1995).

In the second approach, we require a functional form for the concentration probability distribution (e.g., a gamma distribution: Deardorff and Willis, 1988) and estimates of C and the root-mean-square concentration fluctuation σ_c due to an ensemble of meandering puffs. The probability distribution and the σ_c model remain to be selected. The C field including puff meandering is given by Eq. (1), but with $\sigma_{rx}, \sigma_{ry}, \sigma_{rz}$ replaced by the absolute dispersion parameters— $\sigma_x, \sigma_y, \sigma_z$. A Gaussian distribution for C is applicable to the SBL where the probability density function (p.d.f.) of the vertical velocity w is Gaussian. However, for the CBL, a skewed w p.d.f. is more consistent with laboratory and field data. A skewed p.d.f. is adopted here and is parameterized by the superposition of two Gaussian distributions (Weil, 1988).

The C field due to an ensemble of meandering puffs is derived from p_w following the same approach as applied to continuous plumes (Weil, 1988). The resulting expression for C is

$$C = \frac{Q}{(2\pi)^{3/2}\sigma_x\sigma_y} \exp\left(-\frac{(x-Ut)^2}{2\sigma_x^2} - \frac{y^2}{2\sigma_y^2}\right) \times \sum_{j=1}^2 \frac{\lambda_j}{\sigma_{zj}} \exp\left(-\frac{(z-h_c-\bar{z}_j)^2}{2\sigma_{zj}^2}\right) \quad (2)$$

where $\sigma_{zj} = \sigma_j x/U$ and $\bar{z}_j = \bar{w}_j x/U$ with $j = 1, 2$. The λ_j, σ_j , and \bar{w}_j ($j = 1, 2$) are the weight, mean velocity, and standard deviation of each Gaussian p.d.f. comprising p_w . Equation (2) applies for short distances such that the plume interaction with the ground or elevated inversion is weak. The complete expression for C includes multiple cloud reflections at the ground and PBL top.

The time-averaged concentration can be found from the dose where the partial dose is defined by $\psi(x, y, z, t) = \int_0^t C(x, y, z, t') dt'$ and the total dose by $\psi_\infty = \psi(x, y, z, \infty)$. For clouds with short passage times over a receptor, the average concentration \bar{C} can be obtained from $\bar{C} = (\psi(t_2) - \psi(t_1))/T_a$, where the averaging time $T_a = t_2 - t_1$. If the puff passage time $4\sigma_{rx}/U$ is less than T_a , then $\bar{C} = \psi_\infty/T_a$.

Cloud rise and inversion penetration. Scorer (1978) combined theory and laboratory experiments to obtain the following expression for cloud

rise in a neutral environment

$$\Delta h = 2.35(M_T t + F_T t^2)^{1/4} \quad (3)$$

M_T and F_T are the initial momentum and buoyancy of the cloud and are given by

$$M_T = \frac{4\pi}{3} r_o^3 w_o \quad \text{and} \quad F_T = \frac{g Q_T}{c_p \rho_a \Theta_a} \quad (4)$$

where w_o, r_o , and Q_T are the initial velocity, radius, and heat content of the thermal, g is the gravitational acceleration, c_p is the specific heat of air, and ρ_a and Θ_a are the ambient air density and potential temperature.

Scorer also found the puff radius to be $r = \alpha \Delta h_t$, where Δh_t is the cloud top height and α is an empirical entrainment coefficient. α ranged from 0.14 to 0.5 with a mean of 0.25. The relative dispersion $\sigma_r = r/\sqrt{2}$.

Using field observations, Weil (1982) confirmed that Eq. (3) was a good fit to data over a wide range of times. Thus, Eq. (3) is suitable for the initial rise of a cloud, i.e., before it is limited by stable stratification. The Q_T can be determined from the mass of the detonation and its heat content, $H = 1100$ kcal/kg TNT equivalent.

For cloud penetration of an elevated density jump, results have been found from laboratory experiments in a nonturbulent environment. Richards (1961) obtained an empirical expression for the fraction P of the cloud penetrating the jump: $P \approx 1 - 0.5\Delta\rho_i/\Delta\rho_{Ti}$, where $\Delta\rho_i$ is the density jump and $\Delta\rho_{Ti}$ is the average density excess of the cloud when it reaches the jump. The $\Delta\rho_{Ti}$ can be estimated from F_T and r .

The $\Delta\rho$ in a detonation cloud is related to the cloud temperature excess $\Delta\Theta$ by $\Delta\rho/\rho_a = \Delta\Theta/\Theta_a$ with $\Delta\Theta = (3/4\pi)Q_T/(\rho_a c_p r^3)$. We can then rewrite Richards' expression as $P = 1 - (2\pi/3)(\Delta\Theta_i \rho_a c_p \alpha^3 h^3/Q_T)$, where $\Delta\Theta_i$ is the temperature jump at $z = h$. The h_s is assumed to be zero so that the cloud radius at the inversion is αh . The above relationship shows the strong sensitivity of P to αh .

Figure 1 shows examples of P versus the detonation mass W , where we have used $Q_T = W \cdot H$ and $\alpha = 0.25$. For $h = 500$ m, one can see that a significant fraction of the cloud material penetrates the temperature jump for $\Delta\Theta_i = 1$ or 3°C . However, for $h = 1000$ m, the P is significantly reduced.

A more realistic temperature distribution above the CBL is a constant $\partial\Theta_a/\partial z$. Experiments simulating this distribution as well as a jump above a well-mixed layer are currently underway in a salt-stratified tank at the EPA Fluid Modeling Facility in North Carolina.

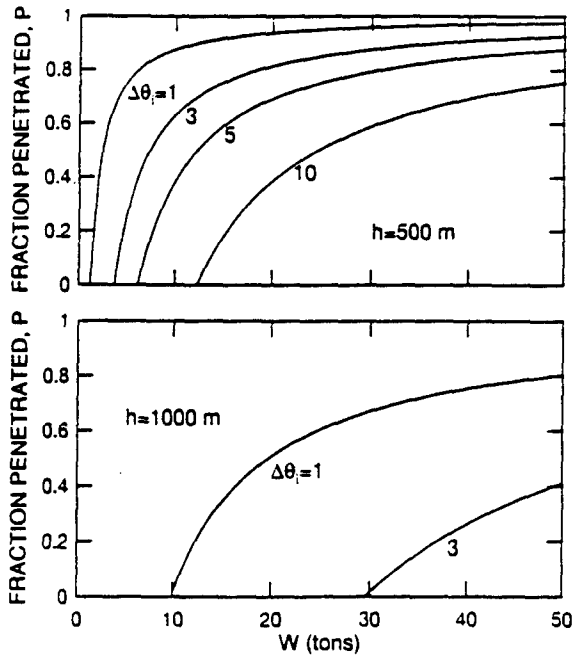


Fig. 1. Fraction of cloud penetrating an elevated temperature jump ($\Delta\theta_i$, °C) as a function of detonation mass.

Dispersion parameters. For clouds, σ_r is dominated by entrainment for short times with $\sigma_r = \sigma_{rb} = 0.18\Delta h$. At intermediate times ($t < T_L$), the σ_r may be dominated by ambient turbulence in the inertial subrange with $\sigma_r \sim \sigma_{ra} = a_1 \epsilon^{1/2} t^{3/2}$, where T_L is the Lagrangian time scale, ϵ is the turbulent kinetic energy dissipation rate, and a_1 is a constant (see Thomson, 1990). At long times ($t \gg T_L$), $\sigma_{ra} = (2\sigma_w^2 T_L t)^{1/2}$ for homogeneous isotropic turbulence. For σ_{ra} , we use an interpolation expression of the form $\sigma_{ra} = a_1 \epsilon^{1/2} t^{3/2} / (1 + a_2 t/T_L)$ to satisfy the intermediate- and long-time results. In addition, ϵ can be written as $\epsilon = b\sigma_w^2/T_L$ in homogeneous isotropic turbulence.

In a strong CBL, the following approximations can be made for $z \geq 0.1h$: $\epsilon \simeq 0.4w_*^3/h$, $\sigma_w \simeq 0.6w_*$, and $T_L \sim 0.7h/w_*$ (Weil, 1988). These approximations coupled with $\epsilon = b\sigma_w^2/T_L$ lead to $b = 0.78$. To satisfy the long-time σ_{ra} limit, we must have $a_2 = 0.62a_1$; a_1 is estimated to be 0.57 from Thomson's two-particle model results. The resulting parameterization for σ_{ra} in the CBL is

$$\frac{\sigma_{ra}}{h} = \frac{0.36X^{3/2}}{1 + 0.51X} \quad \text{with} \quad X = \frac{w_* x}{Uh}, \quad (5)$$

where we have assumed $t = x/U$.

To connect the short-, intermediate-, and long-time relative dispersion regimes in a continuous

manner, we adopt the following parameterization: $\sigma_r^3 = \sigma_{rb}^3 + \sigma_{ra}^3$. For clouds dominated by buoyancy, $\sigma_{rb} = 0.42F_T^{1/4} t^{1/2}$.

The total or absolute dispersion is necessary to estimate the C for a meandering puff or plume. The σ_x and σ_y in Eq. (2) can be obtained from a parameterization of Taylor's theory: $\sigma_x = \sigma_u t / (1 + t/2T_{Lx})^{1/2}$ and similarly for σ_y . The T_{Lx} is the Lagrangian time scale for the u component and can be parameterized by $T_{Lx} \propto \sigma_u/h$, etc. (e.g., see Venkatram and Wyngaard, 1988). For the CBL and the results below, we use $T_{Lx} = T_{Ly} = 0.7h/w_*$ and $\sigma_u = \sigma_v = 0.6w_*$.

3.2 Some Results

We have computed the C_c in the buoyant puff and the mean GLC along $y = 0$ due to a meandering puff for $0.1 \leq W \leq 50$ tons. The σ_r , σ_x , and σ_y were calculated as described above. In the following, the cloud buoyancy is characterized by its dimensionless value

$$F_{T*} = \frac{F_T}{w_*^2 h^2}; \quad (6)$$

we used $w_* = 2$ m/s, $h = 1000$ m, and $U = 5$ m/s.

Figure 2 shows the dimensionless concentration $C_c h^3/Q$ as a function of X . We have neglected cloud penetration of the inversion but included cloud reflection at $z = 0, h$ and assumed that $h_e = \text{Min}(\Delta h, h)$. The large variation in the dimensionless C_c at short range ($X < 1$) is due to the buoyancy-induced dispersion σ_{rb} . As can be seen, $C_c h^3/Q$ decreases systematically and significantly with an increase in F_{T*} due to the increase in σ_{rb} with F_{T*} . For $X > 1$, the curves converge to the same limit because at long times the σ_r is dominated by σ_{ra} , which is independent of F_T .

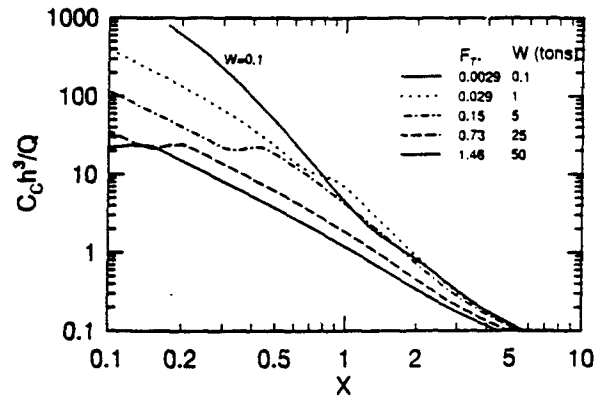


Fig. 2. Dimensionless concentration at cloud centroid versus dimensionless downwind distance.

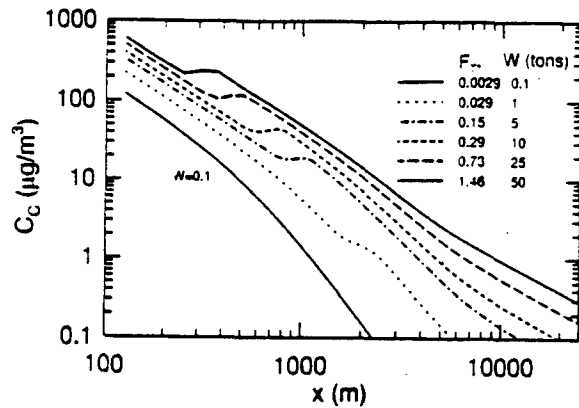


Fig. 3. SO₂ concentration at cloud centroid versus downwind distance.

Figure 3 shows dimensional values of the peak (C_c) SO₂ concentrations in the cloud, with $Q = W \cdot E_f$ where $E_f (= 2.23 \times 10^{-4}$; Andrulis, 1992) is the SO₂ emission factor. In Fig. 3, the order of the curves is reversed from Fig. 1—the curve for $W = 50$ tons exhibits the highest C_c . The reversal is due to the increase in Q with W , which overcomes the decrease in C_c due to the increase in σ_{rb} with F_T . At small x , all of the curves have the same slope: $C_c \propto x^{-3/2}$ because $\sigma_{rb} \propto x^{1/2}$. Some curves exhibit a short region of a nearly constant C_c with x ; this is due to puff trapping in the CBL. At large distances ($x > 10$ km), clouds for all cases become uniformly mixed in the vertical but continue to spread laterally; thus, $C_c \propto Q/\sigma_{ra}^2 \propto Q/x$ as shown.

The dimensionless mean GLC, Ch^3/Q , along the puff centerline is shown in Fig. 4; this mean is for an ensemble of meandering puffs and is obtained from Eq. (2) with reflection terms included. Again, the highest dimensionless concentration occurs for the smallest F_T ; this is attributed to the smaller Δh for the smaller detonations. Likewise, the increase in the distance to the maximum concentration with F_T is due to the increase in Δh . Note that for $X < 1$, the Ch^3/Q can be two orders of magnitude smaller than the $C_c h^3/Q$ (Fig. 2) at the same X value, but at $X \approx 10$, the curves from both figures converge to the same limit. This occurs because the puff becomes uniformly mixed in z and the $\sigma_x, \sigma_y \approx \sigma_{ra}$ at large t or x .

Figure 5 shows the mean dimensional GLC for the same range of W and F_T values as in Figs. 2–4. Several interesting features are found: 1) A non-monotonic variation occurs in the maximum GLC C_m with W and F_T . 2) The variation in C_m for $0.1 \leq W \leq 50$ tons is only about a factor of 4 even though the range in Q is a factor of 500; the weak

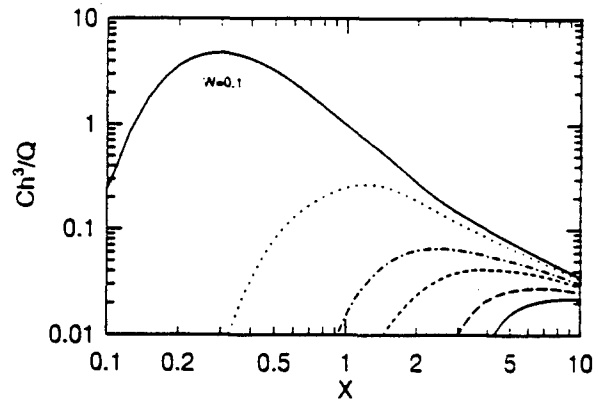


Fig. 4. Dimensionless mean ground-level concentration of cloud versus dimensionless downwind distance; see Fig. 3 for key to lines.

dependence on Q is attributed to the increase in Δh with F_T . 3) The C_m is of the order of $0.1 \mu\text{g}/\text{m}^3$, which is the lower bound for C_c in Fig. 3.

We should clarify again the meaning and use of C in Figs. 4 and 5. It is the mean GLC along $y = 0$ due to an ensemble of meandering puffs and probably has little to do with an observed centerline GLC in an individual puff. This computed C is to be used together with a modeled σ_c in a concentration probability distribution to estimate the peak short-term GLC that could occur downstream of the detonation. The peak GLC would correspond to some specified probability level.

4. SHORT-DURATION RELEASES

4.1 Dispersion Model

For short-duration releases or burns, our general approach is an integrated puff model in which the short-term mean concentration relative to the puff centerline is

$$C = \int_0^{t_r} \frac{Q_r f(t') dt'}{(2\pi)^{3/2} \sigma_{rx} \sigma_{ry} \sigma_{rz}} \quad (7a)$$

$$f = \exp \left[-\frac{(x - U(t - t'))^2}{2\sigma_{rx}^2} - \frac{y^2}{2\sigma_{ry}^2} - \frac{z'^2}{2\sigma_{rz}^2} \right], \quad (7b)$$

where t' is the puff emission time, t_r is the total release duration, Q_r is the continuous source emission rate, $z' = z - h_e$, $\sigma_{rx} = \sigma_{rx}(t - t')$, and similarly for σ_{ry}, σ_{rz} . The integration in (7a) can be carried out analytically for limiting forms of $\sigma_{rx}(t - t')$, etc., but must be done numerically

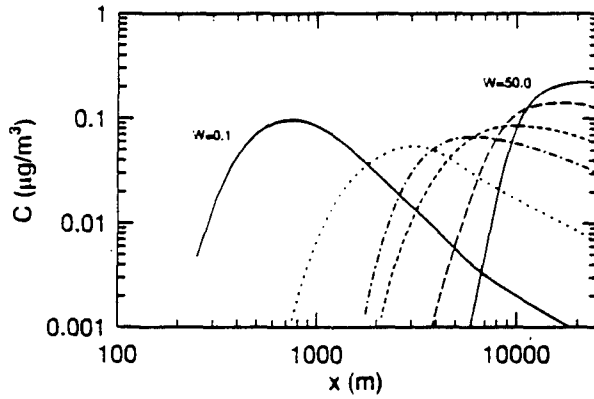


Fig. 5. Mean ground-level SO_2 concentration of cloud versus downwind distance; see Fig. 3 for key to lines.

in general. Numerical integration is required when using the parameterization $\sigma_{rx} = \sigma_{ry} = \sigma_{rz} = \sigma_r = a_1 \epsilon^{1/2} (t - t')^{3/2} / (1 + a_2 (t - t') / T_L)$.

The integrated puff model also can be used for the mean concentration of meandering puffs by replacing the relative dispersion by the absolute dispersion.

In the following, we focus on the C_c for a short-duration release (burn) and consider two limiting cases. 1) For $t < t_r$, we expect the rise and dispersion of the integrated puff to reduce to that of a continuous plume for sufficiently strong winds such that the relative dispersion in the x direction can be neglected. 2) For $t > t_r$, the C field should reduce to that for an instantaneous puff but with $Q = Q_r t_r$ and $F_T = (4\pi/3) F_b t_r$, where $F_b (= w_o r_o^2 g \Delta \Theta_o / \Theta)$ is the continuous source buoyancy flux. As will be shown below, the C_c for the long-time puff solution is lower than that for the plume solution. Thus, we take the plume solution as an upper bound and $C_c = \text{Min}(C_{cpl}, C_{cpu})$, where C_{cpl} and C_{cpu} denote the C_c values for the plume and puff, respectively.

The mean concentration field relative to the plume centerline is given by

$$C = \frac{Q_r}{2\pi U \sigma_{ry} \sigma_{rz}} \exp \left(-\frac{y^2}{2\sigma_{ry}^2} - \frac{(z - h_e)^2}{2\sigma_{rz}^2} \right). \quad (8)$$

Here, the plume rise is attributed to buoyancy and is given by $\Delta h = 1.6 F_b^{1/3} x^{2/3} / U$ and its radius is $r = 0.4 \Delta h$ (Briggs, 1984). Source momentum effects can be included in the future. As with the puff model, we will assume $\sigma_{ry} = \sigma_{rz} = \sigma_r$ and $\sigma_r^3 = \sigma_{rb}^3 + \sigma_{ra}^3$. The σ_{ra} is given by Eq. (5) and the plume $\sigma_{rb} = r / \sqrt{2} = 0.45 F_b^{1/3} x^{2/3} / U$. The $C_c = Q_r / (2\pi U \sigma_r^2)$ from Eq. (8); these expressions can be expanded to include reflection at $z = 0, h$.

To demonstrate the applicability of the instantaneous puff model (Eq. 1) for long times— $t > t_r$ and $t > T_L$, we carry out the integration in Eq. (7a) for $\sigma_{rx} = \sigma_{ry} = \sigma_{rz} = \sigma_r = (2\sigma_w^2 T_L t)^{1/2}$ and assume $\sigma_u = \sigma_v = \sigma_w$. We ignore the dependence of Δh on t' . The result is

$$C = \frac{Q_r}{4\pi \sigma_r^2} \exp \left(\frac{U}{2\sigma_w^2 T_L} (x - r) \right) \times \left[\text{erf} \left(\frac{r - U(t - t_r)}{\sqrt{2}\sigma_r} \right) - \text{erf} \left(\frac{r - Ut}{\sqrt{2}\sigma_r} \right) \right], \quad (9)$$

where erf is the error function and $r^2 = x^2 + y^2 + (z - h_e)^2$. We evaluate this expression at a t corresponding to the center of the cloud, $x = U(t - t_r/2)$, or $t = x/U + t_r/2$. The C_c is found to be $C_c = Q_r t_r / [(2\pi)^{3/2} \sigma_r^3]$. This result supports the use of the instantaneous puff model, with $Q = Q_r t_r$, for the long-time limit of a finite-duration release.

4.2 Some Results

Results are presented for the dimensionless concentration $C_c U h^2 / Q_r$ for the plume and instantaneous puff models, with reflection at $z = 0, h$ included in both. The continuous source buoyancy flux is characterized by its dimensionless value:

$$F_* = \frac{F_b}{U w_*^2 h}. \quad (10)$$

Figure 6 shows the dimensionless C_c for the plume model with F_* in the range $0.001 \leq F_* \leq 0.3$. The trends appear similar to those for the puff model in Fig. 2 although the variation of $C_c U h^2 / Q_r$ with F_* is not as great as for the puff model. For $X < 1$, the decrease in the dimensionless C_c with increasing F_* is due to the increase in σ_{rb} with F_b . For $X > 1$, all of the curves approach the same asymptotic curve; this is due to the dominance of σ_{ra} at large times and its independence of F_b .

Figure 7 presents the dimensionless C_c for both the plume and puff models for $F_* = 0.001$ and 0.01 and various values of $t_{r*} = t_r w_* / h$. The time scale $h/w_* = 500$ s for the w_* ($= 2$ m/s) and h ($= 1000$ m) used here, so that t_r ranges from 50 s to 500 s or about 1 to 8 min. The plume C_c is chosen as long as it exceeds the puff C_c . As can be seen, the distance over which the plume solution applies increases as t_{r*} does.

5. ACKNOWLEDGMENTS

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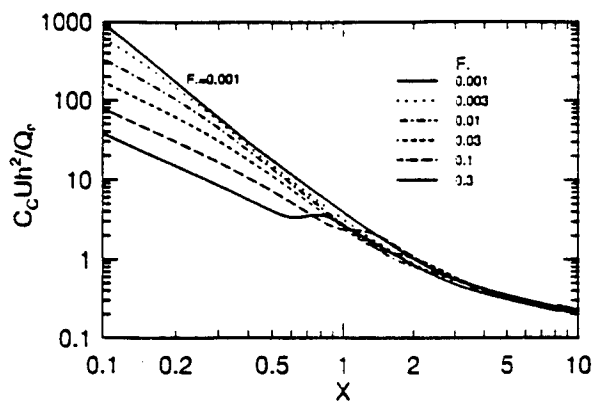


Fig. 6. Dimensionless concentration at plume centroid versus dimensionless downwind distance.

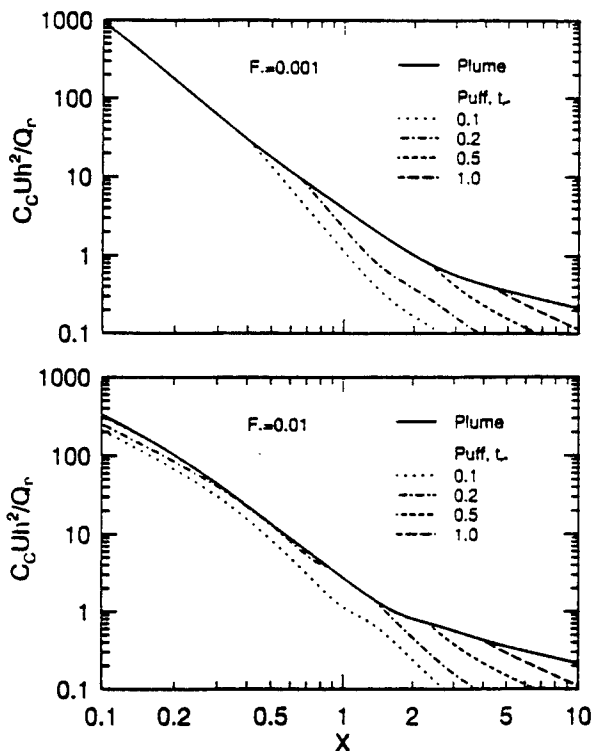


Fig. 7. Dimensionless concentration at plume and puff centroid versus dimensionless downwind distance.

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